Supporting Information for:

Carboberyllation: addition of organoberyllium species to alkenes and alkynes. A comparison with carboboration.

Terri E. Field-Theodore, Shannon A. Couchman, David J. D. Wilson and Jason L. Dutton**

*david.wilson@latrobe.edu.au, j.dutton@latrobe.edu.au

Department of Chemistry and Physics, La Trobe Institute for Molecular Sciences, La Trobe University, Melbourne, Victoria, Australia, 3086

Table of Contents

Table S1. B3LYP/6-311++G(d,p) optimized geometries of alkene, alkyne and beryllium species reactants.

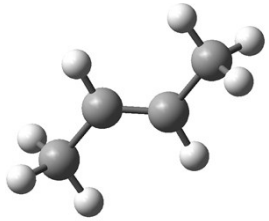
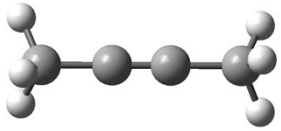
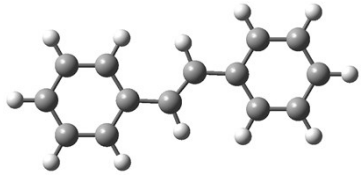
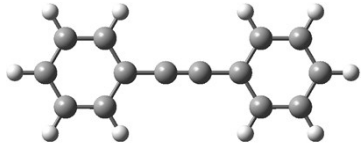
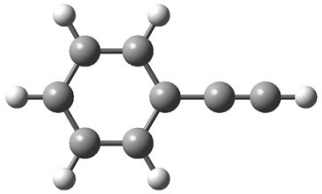
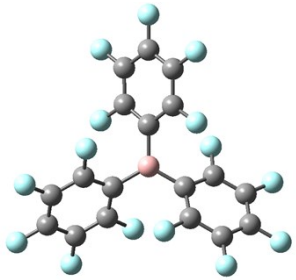
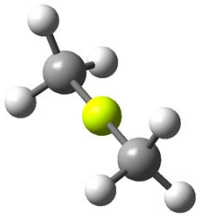
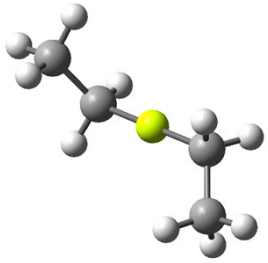
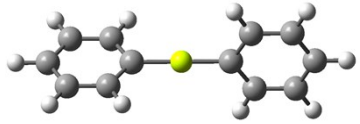
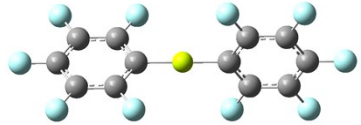
Molecule	***trans*-2-butene**	**2-butyne**	***E*-stilbene**	**Diphenylacetylene**
Reactant alkene/ alkyne				
Molecule	**Phenylacetylene**		**Molecule**	**$B(C_6F_5)_3$**
Reactant alkene/ alkyne			Reactant boron species	
Molecule	**Me-Be-Me**	**Et-Be-Et**	**Ph-Be-Ph**	**C_6F_5-Be-C_6F_5**
Reactant beryllium species				

Table S2. B3LYP/6-311++G(d,p) optimized geometries of 1,1-Be-Me_2 transition states and products.

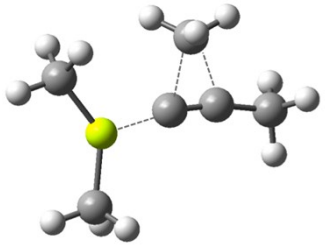
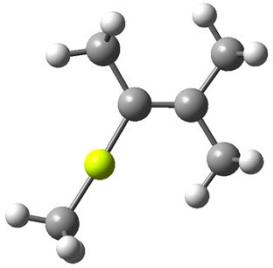
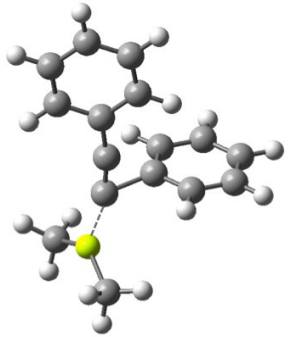
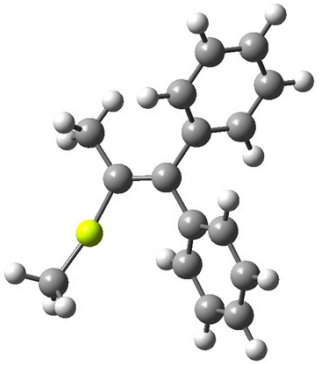
Molecule	Transition State	Product
1,1-Be-Me_2 trans-2-butene		
1,1-Be-Me_2 diphenylacetylene		

Table S3. B3LYP/6-311++G(d,p) optimized geometries of 1,1-Be-Et_2 transition states and products.

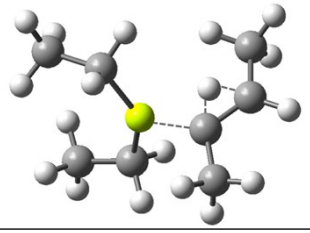
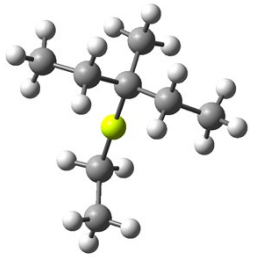
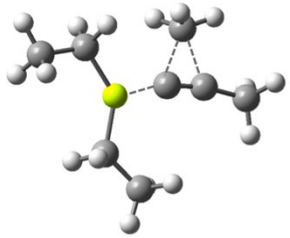
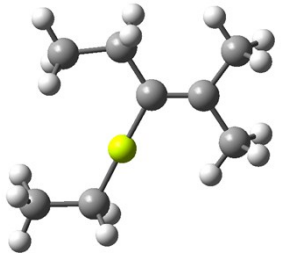
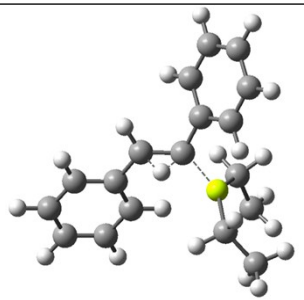
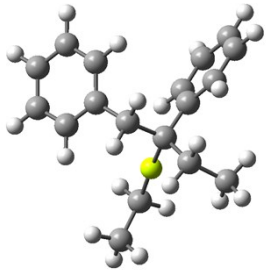
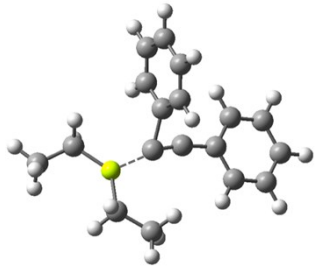
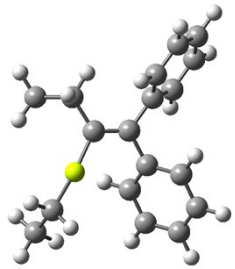
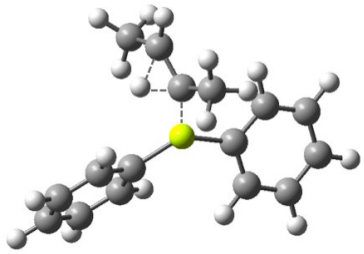
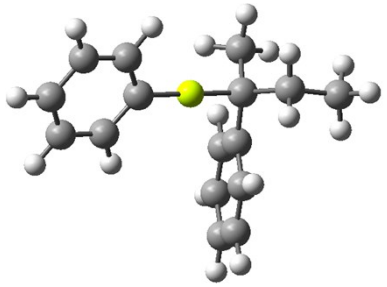
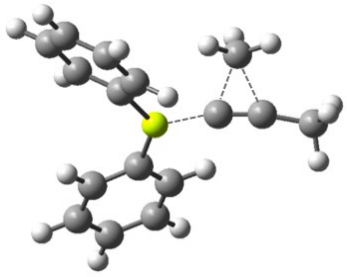
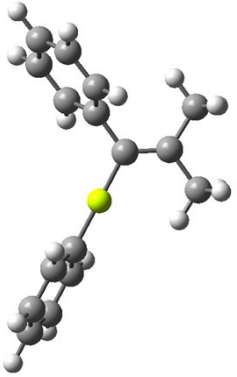
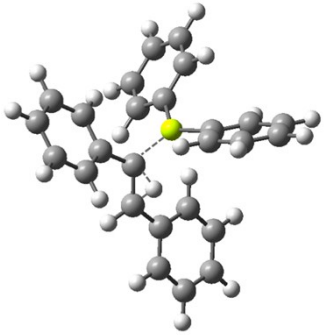
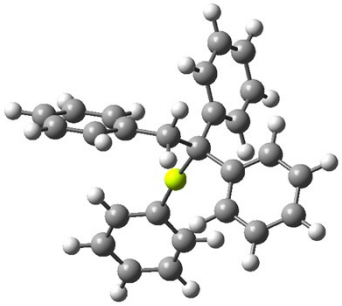
Molecule	Transition State	Product
1,1-Be-Et_2 trans-2-butene		
1,1-Be-Et_2 2-butyne		
1,1-Be-Et_2 *E*-stilbene		
1,1-Be-Et_2 diphenylacetylene		

Table S4. B3LYP/6-311++G(d,p) optimized geometries of 1,1-Be-Ph_2 transition states and products.

Molecule	Transition State	Product
1,1-Be-Ph_2 trans-2-butene		
1,1-Be-Ph_2 2-butyne		
1,1-Be-Ph_2 *E*-stilbene		

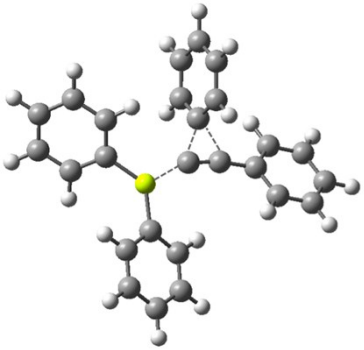
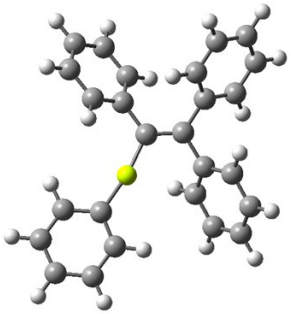
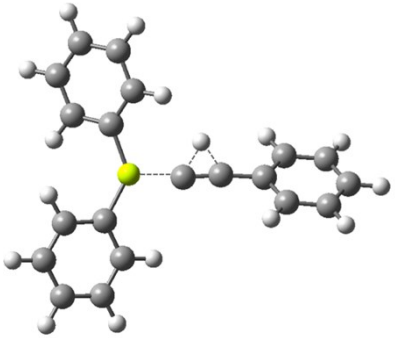
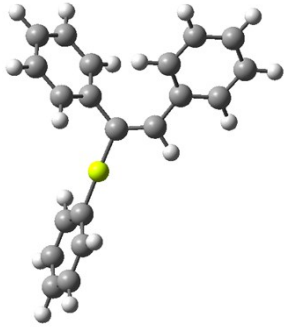
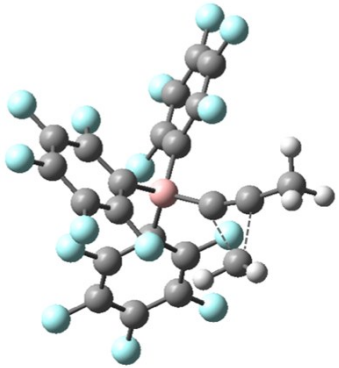
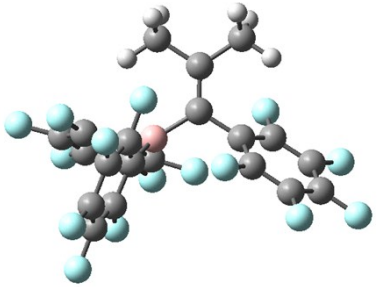
Molecule	Transition State	Product
1,1-Be-Ph_2 diphenylacetylene		
1,1-Be-Ph_2 phenylacetylene		

Table S5. B3LYP/6-311++G(d,p) optimized geometries of 1,1-$B(C_6F_5)_3$ transition states and products.

Molecule	Transition State	Product
1,1-$B(C_6F_5)_3$ 2-butyne		

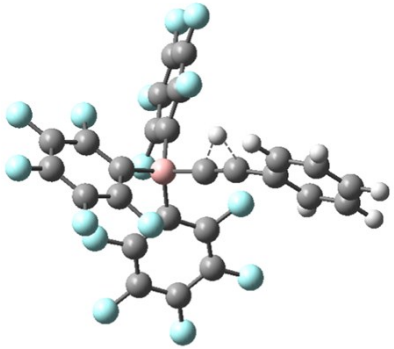
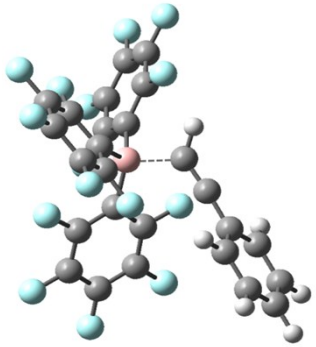
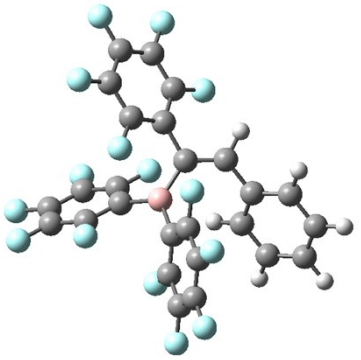
Molecule	Transition State	Adduct	Product
1,1-$B(C_6F_5)_3$ phenylacetylene			

Table S6. B3LYP/6-311++G(d,p) optimized geometries of 1,1-Be(C_6F_5)$_2$ transition states and products.

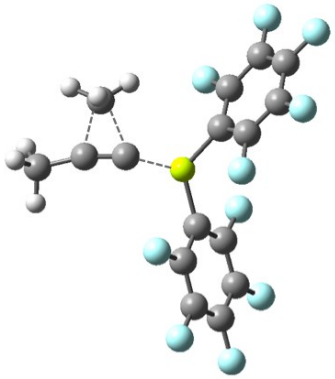
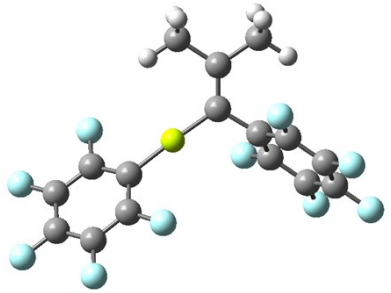
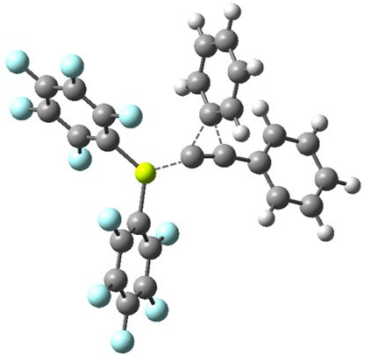
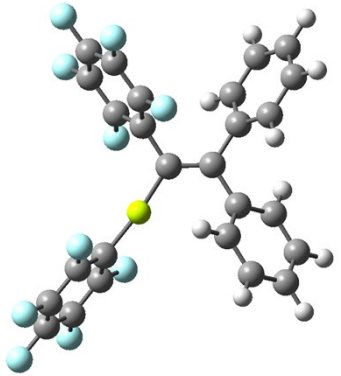
Molecule	Transition State	Product
1,1-Be(C_6F_5)$_2$ 2-butyne		
1,1-Be(C_6F_5)$_2$ diphenylacetylene		

Table S7. B3LYP/6-311++G(d,p) optimized geometries of 1,2-Be-Me_2 transition states and products.

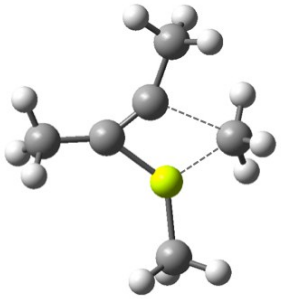
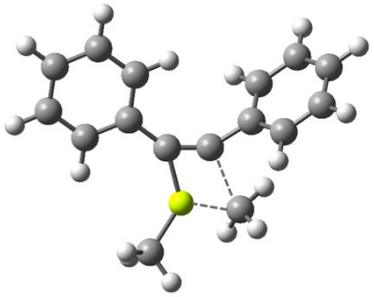
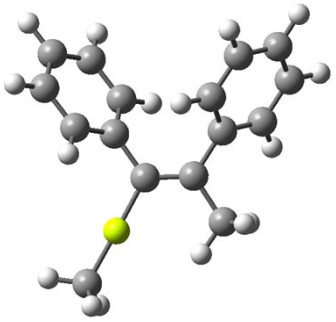
Molecule	Transition State	Product
1,2-Be-Me_2 trans-2-butene		
1,2-Be-Me_2 diphenylacetylene		

Table S8. B3LYP/6-311++G(d,p) optimized geometries of 1,2-Be-Et_2 transition states and products.

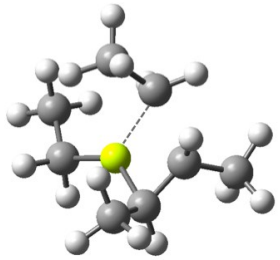
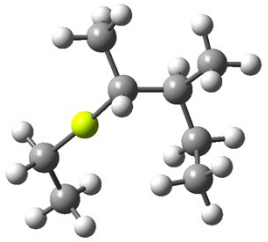
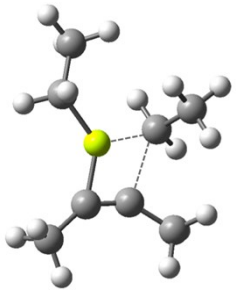
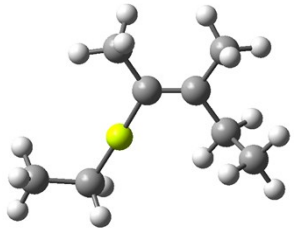
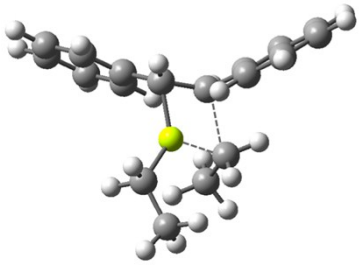
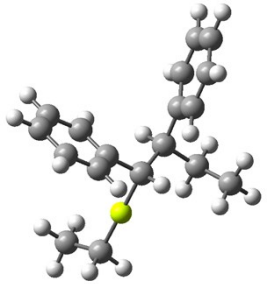
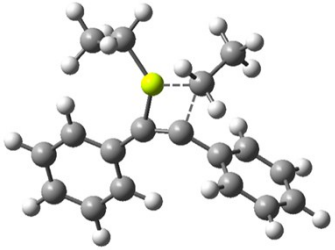
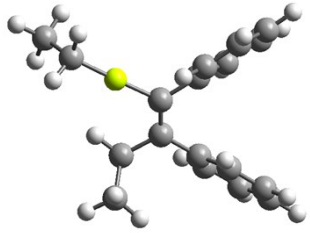
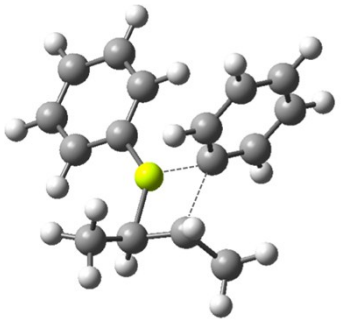
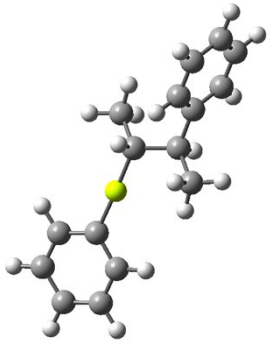
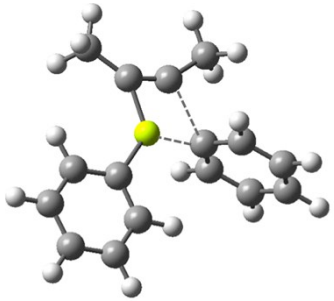
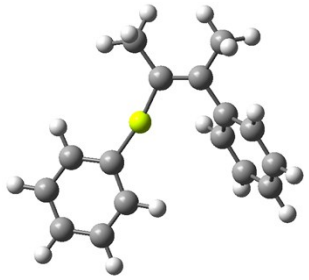
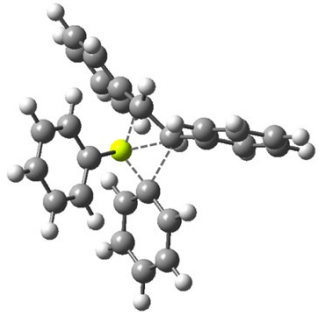
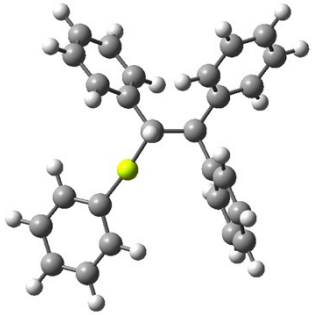
Molecule	Transition State	Product
1,2-Be-Et_2 trans-2-butene		
1,2-Be-Et_2 2-butyne		
1,2-Be-Et_2 *E*-stilbene		
1,2-Be-Et_2 diphenylacetylene		

Table S9. B3LYP/6-311++G(d,p) optimized geometries of 1,2-Be-Ph_2 transition states and products.

Molecule	Transition State	Product
1,2-Be-Ph_2 trans-2-butene		
1,2-Be-Ph_2 2-butyne		
1,2-Be-Ph_2 *E*-stilbene		

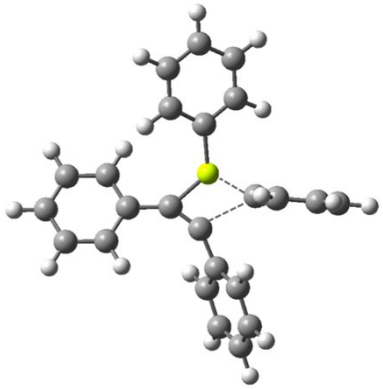
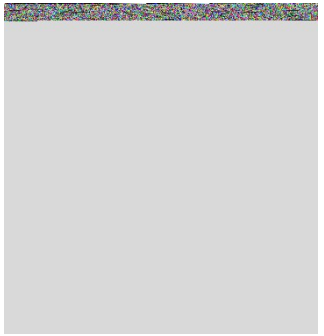
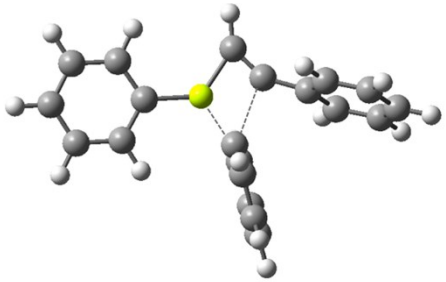
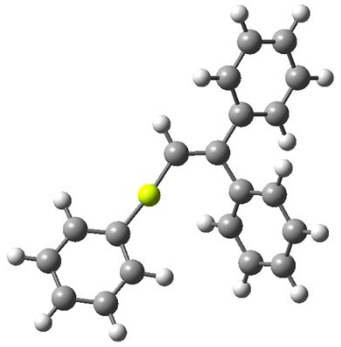
Molecule	Transition State	Product
1,2-Be-Ph_2 diphenylacetylene		
1,2-Be-Ph_2 phenylacetylene		

Table S10. B3LYP/6-311++G(d,p) optimized geometries of 1,2-B(C_6F_5)$_3$ transition states and products.

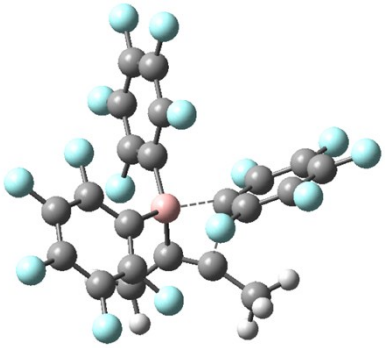
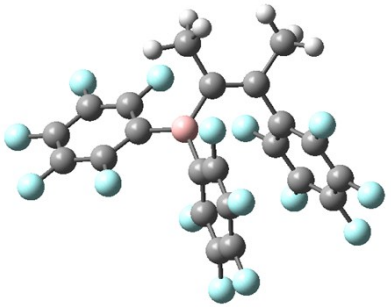
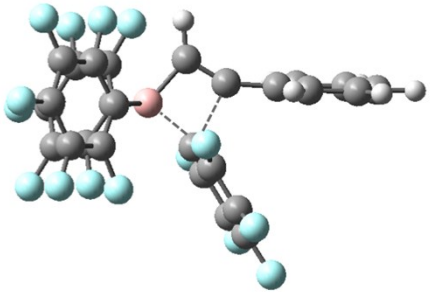
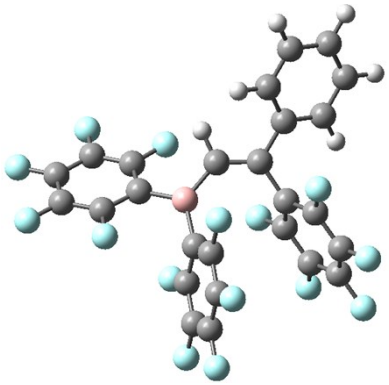
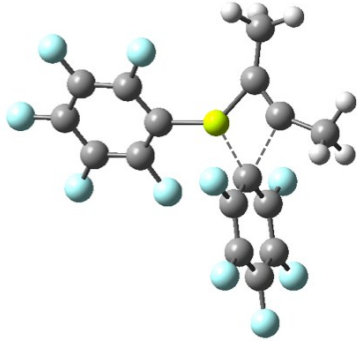
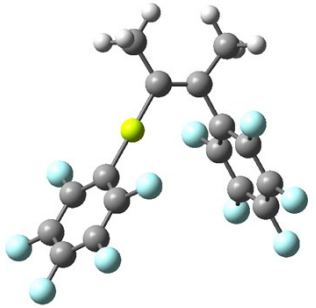
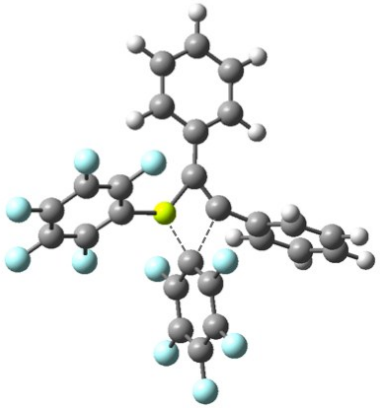
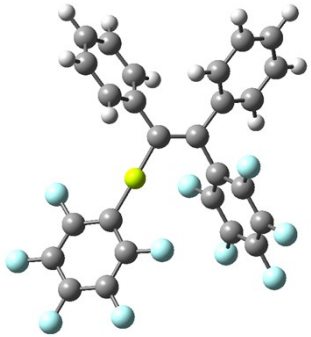
Molecule	Transition State	Product
1,2-B(C_6F_5)$_3$ 2-butyne		
1,2-B(C_6F_5)$_3$ phenylacetylene		

Table S11. B3LYP/6-311++G(d,p) optimized geometries of 1,2-Be(C_6F_5)$_2$ transition states and products.

Molecule	Transition State	Product
1,2-Be(C_6F_5)$_2$ 2-butyne		
1,2-Be(C_6F_5)$_2$ diphenylacetylene		

Cartesian Coordinates

All geometries listed have been optimized at the B3LYP/6-311++G(d,p) level of theory. Coordinates are enumerated in angstroms, and all energies are expressed in Hartrees: SCF (E), zero-point corrected (E_0), thermally corrected (H) and Gibb's Free (G).

Reactants

***trans*-2-butene**

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -157.274609473
E_0 = -157.167265
H = -157.160833
G = -157.194020

0 1

C	0.324262	0.582339	-0.000001
C	-0.324262	-0.582339	-0.000001
H	1.414297	0.571751	-0.000002
H	-1.414297	-0.571751	-0.000002
C	-0.324262	1.936254	0.000001
H	-0.025761	2.518835	0.878885
H	-0.025738	2.518850	-0.878866
H	-1.414344	1.857628	-0.000015
C	0.324262	-1.936254	0.000001
H	0.025738	-2.518850	-0.878866
H	1.414344	-1.857628	-0.000015
H	0.025761	-2.518835	0.878885

2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -156.026849032
E_0 = -155.943067
H = -155.936360
G = -155.971854

0 1

C	-0.602113	0.001711	-0.001635
C	0.602104	0.000845	-0.001228
C	2.060752	-0.000570	0.000673
H	2.455912	-0.863472	-0.543622
H	2.458037	0.902108	-0.472948
H	2.454247	-0.041907	1.020691
C	-2.060806	-0.000674	0.000721
H	-2.456046	-0.676137	-0.763872
H	-2.453236	-0.327092	0.968484
H	-2.458534	0.998627	-0.199922

_E_-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -540.846826232
E_0 = -540.632998
H = -540.620706
G = -540.672951

0 1

C	-0.497148	-0.453232	0.000092
C	0.497148	0.453232	-0.000111
H	-0.241225	-1.509583	0.000276
H	0.241225	1.509583	-0.000280
C	-1.938433	-0.186226	0.000104
C	-2.826575	-1.275608	0.000317
C	-2.491284	1.107814	-0.000086
C	-4.205717	-1.086557	0.000337
H	-2.424199	-2.283584	0.000467
C	-3.867219	1.297428	-0.000065
H	-1.841535	1.974981	-0.000252
C	-4.734099	0.202160	0.000146
H	-4.866842	-1.946096	0.000504
H	-4.268731	2.304862	-0.000216
H	-5.807321	0.354608	0.000164
C	1.938433	0.186226	-0.000117
C	2.826575	1.275608	-0.000202
C	2.491284	-1.107814	-0.000046
C	4.205717	1.086557	-0.000203
H	2.424199	2.283584	-0.000265
C	3.867219	-1.297428	-0.000047
H	1.841535	-1.974981	0.000000
C	4.734099	-0.202160	-0.000122
H	4.866842	1.946096	-0.000265
H	4.268731	-2.304862	0.000006
H	5.807321	-0.354607	-0.000121

Diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -539.598841631
E_0 = -539.408181
H = -539.396166
G = -539.447304

0 1

C	-0.605459	-0.000029	-0.000040
C	0.605459	-0.000010	-0.000035
C	2.028782	-0.000004	-0.000007
C	2.745864	-1.210908	0.004108
C	2.745854	1.210906	-0.004093
C	4.136050	-1.206283	0.004147
H	2.200919	-2.147206	0.007349
C	4.136040	1.206294	-0.004072
H	2.200901	2.147199	-0.007357
C	4.836749	0.000008	0.000052
H	4.674929	-2.147122	0.007419
H	4.674912	2.147137	-0.007321
H	5.920757	0.000013	0.000076
C	-2.028782	-0.000015	-0.000029
C	-2.745844	1.210901	0.004080
C	-2.745874	-1.210912	-0.004123
C	-4.136030	1.206300	0.004104
H	-2.200883	2.147190	0.007326
C	-4.136060	-1.206278	-0.004116
H	-2.200937	-2.147214	-0.007382
C	-4.836749	0.000019	0.000002
H	-4.674894	2.147147	0.007371
H	-4.674947	-2.147112	-0.007371
H	-5.920756	0.000032	0.000016

Phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -308.477328812
E_0 = -308.368218
H = -308.360842
G = -308.398636

0 1

C	2.021990	-0.000148	-0.000080
C	3.227026	0.000088	-0.000143
C	0.593813	-0.000069	-0.000021
C	-0.119198	1.210865	0.000019
C	-0.119324	-1.210928	-0.000006
C	-1.509909	1.206589	0.000080
H	0.427015	2.146352	0.000006
C	-1.510034	-1.206505	0.000048
H	0.426790	-2.146472	-0.000041
C	-2.209622	0.000079	0.000094
H	-2.048933	2.147232	0.000114
H	-2.049157	-2.147092	0.000059
H	-3.293668	0.000135	0.000139
H	4.289503	0.000020	-0.000220

Me-Be-Me

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -94.6184970194
E_0 = -94.547253
H = -94.540672
G = -94.574977

0 1

Be	0.00000000	0.00000000	0.00007000
C	0.00000000	1.67885200	-0.00003800
H	0.29744400	2.09404300	-0.97134000
H	0.69237700	2.09391700	0.74337100
C	0.00000000	-1.67885200	-0.00003800
H	-0.29744400	-2.09404300	-0.97134000
H	-0.69237700	-2.09391700	0.74337100
H	-0.99006400	2.09362100	0.22805900
H	0.99006400	-2.09362100	0.22805900

Et-Be-Et

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -173.252033859
E_0 = -173.122534
H = -173.113625
G = -173.155293

0 1

Be	0.000000	0.000000	0.337030
C	0.000000	1.687313	0.342871
C	-1.176479	2.383472	-0.383480
H	0.948048	2.040070	-0.091254
H	0.032893	2.034992	1.386713
H	-1.103767	3.475362	-0.335444
H	-1.216034	2.111437	-1.443099
H	-2.141791	2.107283	0.052680
C	0.000000	-1.687313	0.342871
C	1.176479	-2.383472	-0.383480
H	-0.948048	-2.040070	-0.091254
H	-0.032893	-2.034992	1.386713
H	1.103767	-3.475362	-0.335444
H	1.216034	-2.111437	-1.443099
H	2.141791	-2.107283	0.052680

Ph-Be-Ph

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -478.175484707
E_0 = -477.993707
H = -477.981957
G = -478.032674

0 1

Be	0.000000	0.000042	-0.000049
C	-1.675540	0.000067	0.000003
C	-2.417125	0.849219	-0.848770
C	-2.417037	-0.849152	0.848786
C	-3.811258	0.852915	-0.852518
H	-1.900104	1.525485	-1.524682
C	-3.811172	-0.852981	0.852547
H	-1.899948	-1.525360	1.524704
C	-4.511007	-0.000069	0.000015
H	-4.351770	1.518258	-1.517552
H	-4.351613	-1.518374	1.517589
H	-5.595742	-0.000124	0.000014
C	1.675540	-0.000009	-0.000082
C	2.417127	-0.849152	-0.848861
C	2.417035	0.849141	0.848773
C	3.811259	-0.852900	-0.852551
H	1.900106	-1.525350	-1.524840
C	3.811171	0.852905	0.852604
H	1.899946	1.525342	1.524698
C	4.511007	0.000005	0.000062
H	4.351773	-1.518223	-1.517605
H	4.351610	1.518236	1.517710
H	5.595742	0.000005	0.000116

(C_6F_5)-Be-(C_6F_5)

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1470.81517774
E_0 = -1470.714115
H = -1470.693582
G = -1470.765138

0 1

Be	0.000000	0.000062	0.000022
C	-1.677865	0.000028	0.000035
C	-2.414562	-0.834692	0.834931
C	-2.414562	0.834730	-0.834883
C	-3.801859	-0.853993	0.854213
C	-3.801857	0.854002	-0.854198
C	-4.494882	-0.000001	0.000003
C	1.677864	0.000067	0.000047
C	2.414502	-0.834964	-0.834594
C	2.414622	0.835037	0.834640
C	3.801796	-0.854320	-0.853933
C	3.801920	0.854268	0.853884
C	4.494882	-0.000057	-0.000044
F	1.761226	1.670661	1.669889
F	4.477582	1.669257	1.668513
F	5.826047	-0.000111	-0.000087
F	4.477335	-1.669368	-1.668604
F	1.760969	-1.670531	-1.669801
F	-1.761100	-1.670002	1.670445
F	-4.477459	-1.668743	1.669131
F	-5.826047	-0.000020	-0.000019
F	-4.477458	1.668726	-1.669141
F	-1.761094	1.670032	-1.670403

$B(C_6F_5)_3$

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2208.92672205
E_0 = -2208.773681
H = -2208.743849
G = -2208.835788

0 1

B	-0.000261	-0.001237	-0.000933
C	-1.276750	-0.911885	0.000279
C	-1.360905	-2.080261	-0.766667
C	-2.408300	-0.609876	0.767644
C	-2.486726	-2.889801	-0.788826
C	-3.541360	-1.409181	0.789791
C	-3.581429	-2.553484	0.000330
C	-0.150498	1.559793	-0.000457
C	0.674561	2.388735	0.769276
C	-1.118534	2.216714	-0.769542
C	0.547800	3.769589	0.792077
C	-1.257934	3.596337	-0.790864
C	-0.421925	4.376302	0.000984
C	1.427112	-0.650846	-0.001529
C	1.734501	-1.777949	0.769967
C	2.478565	-0.141097	-0.772787
C	2.994627	-2.356649	0.793028
C	3.743813	-0.708486	-0.794040
C	4.003546	-1.820229	0.000207
F	-0.549621	5.699436	0.001737
F	-2.180968	4.180639	-1.557693
F	1.342155	4.518644	1.559764
F	1.619841	1.852088	1.558797
F	-1.943512	1.509986	-1.559946
F	-2.416978	0.478807	1.554687
F	-4.588433	-1.093772	1.554989
F	-4.664193	-3.324572	0.000184
F	-2.530649	-3.982679	-1.553728
F	-0.335030	-2.444426	-1.553821
F	0.798098	-2.328364	1.560588
F	3.248366	-3.417213	1.562602
F	5.214062	-2.369514	0.001196
F	4.710089	-0.201520	-1.562632
F	2.276808	0.924662	-1.565452

Products (Me-Be-Me)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -250.683564819
E_0 = -250.522545
H = -250.510664
G = -250.560136

0 1

C	-0.01834100	0.57866000	0.00033000
C	0.93474200	-0.38287400	0.00004200
C	0.36301700	2.05837100	0.00025100
H	0.95196800	2.33323200	-0.88255000
H	-0.51843000	2.70640300	0.00122600
H	0.95365700	2.33289300	0.88202200
C	2.42288600	-0.12115800	-0.00060600
H	2.89470300	-0.58047100	-0.87797900
H	2.67057600	0.93969400	-0.00147700
H	2.89527000	-0.57915900	0.87715500
Be	-1.63153700	0.13298600	0.00048500
C	0.59169200	-1.85617300	0.00042000
H	1.01195500	-2.35981100	-0.87862300
H	-0.48762700	-2.04013300	0.00101900
C	-3.26741600	-0.25638700	-0.00025200
H	-3.57524200	-0.77441900	0.91679300
H	-3.54159700	-0.90948900	-0.83839600
H	1.01277000	-2.35951300	0.87924100
H	-3.90133500	0.63619000	-0.08149100

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -250.683564819
E_0 = -250.522545
H = -250.510664
G = -250.560136

0 1

C	-0.01834100	0.57866000	0.00033000
C	0.93474200	-0.38287400	0.00004200
C	0.36301700	2.05837100	0.00025100
H	0.95196800	2.33323200	-0.88255000
H	-0.51843000	2.70640300	0.00122600
H	0.95365700	2.33289300	0.88202200
C	2.42288600	-0.12115800	-0.00060600
H	2.89470300	-0.58047100	-0.87797900
H	2.67057600	0.93969400	-0.00147700
H	2.89527000	-0.57915900	0.87715500
Be	-1.63153700	0.13298600	0.00048500
C	0.59169200	-1.85617300	0.00042000
H	1.01195500	-2.35981100	-0.87862300
H	-0.48762700	-2.04013300	0.00101900
C	-3.26741600	-0.25638700	-0.00025200
H	-3.57524200	-0.77441900	0.91679300
H	-3.54159700	-0.90948900	-0.83839600
H	1.01277000	-2.35951300	0.87924100
H	-3.90133500	0.63619000	-0.08149100

Products (Me-Be-Me)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.250133540
E_0 = -633.982419
H = -633.964919
G = -634.027955

0 1

C	-0.34593400	1.88249400	-0.14291000
C	0.06572900	0.58704600	-0.08442100
Be	-1.99504000	2.18053600	0.05931300
C	-3.56989100	2.69749400	0.34281400
H	-3.60853300	3.71115500	0.76151400
H	-4.09033100	2.04281900	1.05320600
C	1.49181900	0.13734600	-0.06463600
C	1.94555700	-0.82656200	-0.97825900
C	2.40583100	0.64398000	0.86987400
C	3.27211700	-1.24866300	-0.97509800
H	1.25113400	-1.24265000	-1.69991900
C	3.73104800	0.21248900	0.88380000
H	2.06934000	1.37065100	1.60034700
C	4.17082400	-0.73125100	-0.04231000
H	3.60408200	-1.98525300	-1.69862200
H	4.41886600	0.61205500	1.62108300
H	5.20239700	-1.06500600	-0.03443700
C	0.62165300	3.04027800	-0.31022000
H	0.72211700	3.61415500	0.61947000
H	1.62453100	2.73292000	-0.61731900
C	-0.95702400	-0.50162600	-0.02656500
C	-0.84849900	-1.55185500	0.90131800
C	-2.07484500	-0.48872300	-0.87672000
C	-1.83984100	-2.52110500	1.00293200
H	0.01466500	-1.59354800	1.55581700
C	-3.07032900	-1.46241500	-0.77585900
H	-2.13685800	0.26331400	-1.65688700
C	-2.95909700	-2.47825800	0.16810100
H	-1.74299100	-3.31317900	1.73746300
H	-3.92067300	-1.43336000	-1.44816300
H	-3.72787800	-3.23860100	0.24635300
H	-4.17876600	2.71136100	-0.57013000
H	0.24433700	3.74701200	-1.05806500

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.250769038
E_0 = -633.983176
H = -633.965590
G = -634.029797

0 1

C	-1.00677000	1.02534000	-0.00740600
C	0.25549900	1.52552700	-0.03575400
Be	-2.33272800	2.05936300	0.01064900
C	0.50562200	3.02004600	-0.04742100
H	1.09180700	3.33667900	0.82155700
H	-0.42598400	3.59472500	-0.03825200
C	-3.67361200	3.06906800	0.03523400
H	-4.61094400	2.50207000	0.10062200
H	-3.74615500	3.69075700	-0.86605600
C	-1.30998300	-0.43287700	0.08610300
C	-2.18816000	-1.03048900	-0.83348300
C	-0.81335100	-1.23334900	1.12829100
C	-2.53126400	-2.37765000	-0.73737100
H	-2.59367500	-0.43351200	-1.64542600
C	-1.16365500	-2.57658700	1.23263600
H	-0.14914400	-0.79264600	1.86271600
C	-2.02054400	-3.15808500	0.29808000
H	-3.20155800	-2.81550700	-1.46922400
H	-0.76682700	-3.17190600	2.04802200
H	-2.29159200	-4.20458700	0.38015000
C	1.49847800	0.69709300	-0.10259200
C	2.55940000	0.91017100	0.79047900
C	1.65398100	-0.28645200	-1.09030700
C	3.72469100	0.15045100	0.71506600
H	2.46887700	1.66268600	1.56616700
C	2.82440000	-1.03523400	-1.17683500
H	0.85122900	-0.45917400	-1.79668100
C	3.86330300	-0.82409300	-0.27144900
H	4.52541500	0.32247700	1.42606900
H	2.92460700	-1.78561500	-1.95337000
H	4.77261600	-1.41105700	-0.33583200
H	-3.66413700	3.75581600	0.89101200
H	1.07816900	3.31405700	-0.93367900

Products (Et-Be-Et)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -330.539051496
E_0 = -330.296998
H = -330.282705
G = -330.337528

0 1

Be	-0.82150300	-0.18947400	0.39724300
C	0.83123500	0.08056000	0.05310900
C	0.99285000	1.38933900	-0.76924800
C	1.64468600	0.19641400	1.36547900
H	1.30148500	1.01764300	2.00152600
H	1.59337400	-0.71256400	1.97192300
H	2.70800700	0.37954200	1.14559400
C	0.40288300	2.65918500	-0.14091700
H	0.54103600	3.52109400	-0.80001600
H	-0.67470100	2.56225600	0.04042500
H	0.87560000	2.90245500	0.81396800
C	-2.45662200	-0.44611700	0.72406700
C	-3.44140100	-0.21145000	-0.44714200
H	-2.74880200	0.19370300	1.57091200
H	-2.58598200	-1.47202100	1.10117500
H	-4.48142000	-0.39208300	-0.15488500
H	-3.38812900	0.81584300	-0.82170900
H	-3.22784400	-0.87098000	-1.29438400
H	0.53829200	1.24741100	-1.75812200
H	2.06508300	1.55797200	-0.95975600
C	1.40105600	-1.08203200	-0.80540700
H	2.47041000	-0.89291100	-0.99284100
H	0.92283200	-1.06285900	-1.79313000
C	1.24968500	-2.49264900	-0.22021400
H	1.65672300	-3.24398500	-0.90304800
H	1.77582000	-2.60094400	0.73162600
H	0.19799800	-2.75117100	-0.04660200

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -330.540546645
E_0 = -330.298096
H = -330.283933
G = -330.338739

0 1

Be	-1.204339	0.747031	0.252980
C	0.479501	0.943507	0.366701
C	1.298888	-0.005605	-0.553313
C	0.781007	-1.463635	-0.520001
C	0.853154	2.434031	0.159245
H	0.679155	2.749683	-0.876077
H	0.260048	3.096151	0.799738
H	1.904661	2.642489	0.386005
C	2.813820	0.047029	-0.283819
H	3.355619	-0.641745	-0.940789
H	3.218484	1.046592	-0.457098
H	3.045023	-0.225398	0.750771
C	0.868740	-2.178483	0.834581
H	1.337558	-2.048025	-1.262637
H	-0.264035	-1.477252	-0.861043
H	0.480881	-3.198073	0.757537
H	1.900472	-2.247836	1.188740
H	0.289239	-1.666348	1.608100
C	-2.888004	0.649858	0.183675
C	-3.499646	-0.656356	-0.377161
H	-3.260572	1.501229	-0.406601
H	-3.287031	0.825894	1.194614
H	-4.594672	-0.630520	-0.382253
H	-3.179179	-0.843825	-1.406949
H	-3.202658	-1.529058	0.213112
H	1.148476	0.340780	-1.586256
H	0.741132	0.695060	1.409717

Products (Et-Be-Et)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -329.324159009
E_0 = -329.105236
H = -329.091155
G = -329.145663

0 1

C	0.58757800	0.25072100	0.00000000
C	1.67229900	-0.56085600	-0.00003400
C	0.74054300	1.77099500	-0.00010800
H	1.32024100	2.09081000	-0.87560000
H	1.32083700	2.09090700	0.87494900
C	3.10718200	-0.08537300	-0.00021700
H	3.63999800	-0.47164100	-0.87786000
H	3.19965000	0.99987000	-0.00023600
H	3.64023800	-0.47164000	0.87728100
Be	-0.92217600	-0.48403900	0.00014100
C	1.55211200	-2.06963700	0.00011100
H	2.04326600	-2.50438300	-0.87888800
H	0.51321200	-2.41588300	0.00011900
C	-2.42222900	-1.26372700	0.00034400
C	-3.68098900	-0.36377800	-0.00046100
H	-2.46694500	-1.93687800	0.87031600
H	-2.46667700	-1.93805700	-0.86872100
H	-4.60757300	-0.94829300	-0.00016800
H	-3.71321200	0.28810400	0.87840100
H	-3.71297800	0.28684800	-0.88026200
H	2.04321600	-2.50419700	0.87923300
C	-0.59535200	2.52354800	0.00030400
H	-1.19276000	2.27606800	-0.88437200
H	-1.19217500	2.27612800	0.88539000
H	-0.44650300	3.60703600	0.00021300

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -329.323356400
E_0 = -329.104578
H = -329.090297
G = -329.145685

0 1

C	0.115395	0.865954	-0.018466
C	1.304893	0.252272	-0.227105
C	0.062430	2.362523	0.276261
H	0.468863	2.958628	-0.550347
H	-0.960119	2.713812	0.441994
H	0.636646	2.626270	1.172254
C	2.636898	0.971625	-0.191570
H	3.365153	0.494387	-0.854560
H	2.544623	2.018648	-0.485624
H	3.068296	0.958394	0.817105
Be	-1.290263	-0.040249	-0.094739
C	1.397461	-1.238081	-0.493367
C	2.145219	-2.024120	0.597741
H	1.903826	-1.401913	-1.454462
H	0.391477	-1.663556	-0.607944
H	2.173728	-3.090666	0.357997
H	3.178105	-1.681959	0.703089
H	1.653385	-1.907004	1.567685
C	-2.736603	-0.911659	-0.168389
C	-4.033394	-0.114532	0.113748
H	-2.678465	-1.757580	0.533247
H	-2.816631	-1.382886	-1.159794
H	-4.928560	-0.742466	0.045780
H	-4.027570	0.326674	1.115729
H	-4.165497	0.708317	-0.596307

Products (Et-Be-Et)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -714.101713905
E_0 = -713.753959
H = -713.733468
G = -713.804816

0 1

Be	-0.09336500	-1.79610900	-0.51953300
C	0.65425700	-0.82293500	0.68026900
C	1.55621700	-1.76250300	1.53550800
C	2.65241800	-2.50226200	0.75829500
H	3.23010600	-3.15296200	1.42088000
H	2.23115900	-3.13667700	-0.03076900
H	3.34825300	-1.80797300	0.28158100
C	-0.76999200	-2.84970300	-1.64859000
C	-1.46385500	-4.11712600	-1.09354300
H	0.01584300	-3.15367800	-2.35681300
H	-1.48979100	-2.28781000	-2.26249400
H	-1.87619600	-4.74473600	-1.89086600
H	-0.77065900	-4.74189200	-0.52107000
H	-2.29358200	-3.86603100	-0.42460500
H	0.91033000	-2.50353100	2.02331800
H	2.01621100	-1.20458500	2.36322600
C	-0.40784400	-0.19728400	1.65555100
H	0.11147900	0.45509000	2.36979700
H	-0.84519700	-1.01082700	2.24592500
C	-1.53016600	0.57569000	0.99831700
C	-2.68456000	-0.08307300	0.55454000
C	-1.44629800	1.95911100	0.80244300
C	-3.71714400	0.61176400	-0.07337300
H	-2.78801200	-1.15242300	0.71933900
C	-2.47666100	2.65974400	0.17779400
H	-0.56421300	2.49100300	1.14200800
C	-3.61521800	1.98861300	-0.26544900
H	-4.60352500	0.08031200	-0.40235700
H	-2.39013500	3.73189600	0.03865400
H	-4.41817300	2.53373500	-0.74885800
C	1.45460500	0.29863900	0.00984000
C	1.10924400	0.76350900	-1.26785100
C	2.53131400	0.93615300	0.64770700
C	1.80114500	1.80364100	-1.88773000
H	0.26872700	0.31790200	-1.79548400
C	3.22860100	1.97608300	0.03680900
H	2.83665500	0.61839600	1.63843200
C	2.86870300	2.41532500	-1.23680800
H	1.50335500	2.13327400	-2.87711800
H	4.05805600	2.44381200	0.55686200
H	3.41418300	3.22182400	-1.71382400

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -714.107698444
E_0 = -713.759311
H = -713.738915
G = -713.810546

0 1

Be	2.240472	-1.309100	-0.377995
C	0.712668	-0.577179	-0.548124
C	-0.404143	-1.187163	0.337019
C	-0.581833	-2.710281	0.076378
C	-1.037968	-3.107797	-1.331073
H	-1.304995	-3.095518	0.802827
H	0.369416	-3.210973	0.302492
H	-1.166969	-4.191718	-1.395873
H	-1.994328	-2.644221	-1.584579
H	-0.312357	-2.821232	-2.097408
C	3.755459	-2.023849	-0.197572
C	4.440495	-1.851091	1.180217
H	4.423932	-1.632828	-0.979611
H	3.668452	-3.097194	-0.423794
H	5.418990	-2.341693	1.216698
H	4.599668	-0.795924	1.422165
H	3.838289	-2.277752	1.988823
H	-0.083778	-1.118106	1.383461
H	0.431962	-0.683682	-1.604091
C	1.029449	0.886882	-0.312122
C	1.370604	1.720106	-1.391685
C	1.073403	1.451330	0.973922
C	1.735539	3.050072	-1.200273
H	1.339020	1.317929	-2.400432
C	1.434070	2.783196	1.167955
H	0.812575	0.849329	1.837364
C	1.769017	3.591790	0.083716
H	1.986236	3.666279	-2.057159
H	1.450347	3.190637	2.173193
H	2.047720	4.628107	0.236278
C	-1.750286	-0.465540	0.268153
C	-2.576210	-0.448311	1.399536
C	-2.222243	0.153081	-0.893929
C	-3.831941	0.154154	1.372584
H	-2.227777	-0.911423	2.318492
C	-3.479052	0.756543	-0.928884
H	-1.601787	0.177649	-1.781742
C	-4.290643	0.758676	0.203244
H	-4.448536	0.156952	2.264990
H	-3.820704	1.231671	-1.842156
H	-5.265589	1.232395	0.177655

Products (Et-Be-Et)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -712.890911793
E_0 = -712.565766
H = -712.545638
G = -712.615682

0 1			
C	-0.36150700	-1.42510300	-0.17963400
C	0.30851400	-0.24531000	-0.07009200
Be	-2.02569200	-1.32443000	-0.46216100
C	-3.65223100	-1.43666200	-0.90680600
C	-4.70715900	-1.28644300	0.21387800
H	-3.80599100	-2.40199400	-1.41364600
H	-3.85020500	-0.68488900	-1.68582400
H	-5.73110800	-1.38186900	-0.16410400
H	-4.58234700	-2.04506000	0.99374900
H	-4.63661600	-0.30960400	0.70280100
C	1.79564700	-0.09790900	-0.01535900
C	2.39724700	0.64764600	1.01042200
C	2.62590800	-0.67585300	-0.98612100
C	3.78059500	0.78775800	1.07823500
H	1.77248400	1.11507600	1.76358300
C	4.01029500	-0.52521400	-0.92795600
H	2.17945600	-1.23453700	-1.80058100
C	4.59342100	0.20252300	0.10753300
H	4.22466500	1.35751800	1.88719200
H	4.63266600	-0.97448200	-1.69419600
H	5.67050800	0.31735500	0.15543200
C	0.33248700	-2.77667900	-0.13003100
H	0.35138400	-3.21454500	-1.13753700
H	1.37773400	-2.68242900	0.17918800
C	-0.38114100	-3.76394500	0.80904900
H	-0.40171500	-3.38335700	1.83434000
H	-1.41723200	-3.94035400	0.49938200
H	0.12717900	-4.73244800	0.82070300
C	-0.46932900	1.03002800	-0.00475000
C	-0.11247800	2.14211100	-0.78689100
C	-1.60095000	1.14269100	0.81977900
C	-0.88181100	3.29995000	-0.77652100
H	0.76772500	2.08591900	-1.41717200
C	-2.37241600	2.30630700	0.83256400
H	-1.84584500	0.33001400	1.49644900
C	-2.01903500	3.38638300	0.03019900
H	-0.59655500	4.13935800	-1.40127400
H	-3.23659400	2.37126000	1.48441900
H	-2.61317300	4.29310300	0.04074500

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -712.891361809
E_0 = -712.566112
H = -712.546002
G = -712.616177

0 1			
C	0.993844	-0.166179	-0.078605
C	0.057447	-1.147175	0.002463
Be	2.625699	-0.569013	-0.157621
C	0.465381	-2.612310	0.001593
C	0.009313	-3.381626	-1.249144
H	0.055874	-3.108021	0.889832
H	1.556118	-2.691354	0.095892
H	0.320323	-4.428428	-1.193588
H	-1.077713	-3.357534	-1.354180
H	0.443106	-2.945876	-2.153606
C	4.271539	-0.930931	-0.234727
C	4.908894	-1.542493	1.036308
H	4.815830	-0.011823	-0.500128
H	4.447662	-1.606666	-1.085399
H	5.977555	-1.744510	0.905900
H	4.810944	-0.875212	1.898344
H	4.435101	-2.490350	1.311513
C	0.670623	1.289623	-0.024331
C	1.163220	2.156086	-1.014576
C	-0.048508	1.858350	1.040046
C	0.920708	3.527370	-0.964112
H	1.729643	1.745244	-1.845538
C	-0.282147	3.229492	1.098482
H	-0.424572	1.215853	1.827660
C	0.195873	4.071548	0.094426
H	1.302215	4.170266	-1.750079
H	-0.839758	3.642641	1.932224
H	0.011639	5.138926	0.140752
C	-1.418758	-0.908661	0.048451
C	-2.212696	-1.489844	1.048717
C	-2.053518	-0.125782	-0.926577
C	-3.589016	-1.277470	1.086510
H	-1.749701	-2.098946	1.817491
C	-3.430877	0.075238	-0.898784
H	-1.459783	0.324673	-1.712675
C	-4.204646	-0.495706	0.110512
H	-4.180406	-1.724574	1.878137
H	-3.900272	0.679854	-1.667030
H	-5.276654	-0.335300	0.135039

Products (Ph-Be-Ph)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -635.460541101
E_0 = -635.167337
H = -635.149899
G = -635.214076

0 1

Be	0.58503400	0.74262400	0.14804600
C	-1.03749900	1.24864500	0.26598600
C	-1.28710600	1.91748900	1.63597400
H	-0.86080600	1.35217200	2.47082700
H	-0.82749100	2.91009600	1.65785100
H	-2.35475400	2.04780000	1.85340700
C	-1.43311000	2.22251300	-0.88462600
H	-1.12863400	1.81528200	-1.85431100
H	-0.85153600	3.14448400	-0.76419400
C	-2.92550700	2.58267100	-0.95744400
H	-3.11788900	3.25389700	-1.79979100
H	-3.54339100	1.69114300	-1.09330200
H	-3.26556700	3.08998300	-0.05103700
C	-1.70554900	-0.11678900	0.13323000
C	-1.69077500	-0.80406000	-1.09910800
C	-2.29351100	-0.78633900	1.22178300
C	-2.23790100	-2.07586800	-1.23676900
H	-1.24913200	-0.33388800	-1.97168600
C	-2.84067200	-2.06220100	1.08560300
H	-2.33642200	-0.30687500	2.19121900
C	-2.81886300	-2.71653200	-0.14273600
H	-2.21015000	-2.56776700	-2.20321600
H	-3.29020600	-2.54266200	1.94824400
H	-3.24570300	-3.70736300	-0.24762900
C	2.17837700	0.22938800	0.05351100
C	2.51535300	-1.13994400	-0.00258800
C	3.25113100	1.14597400	0.03515500
C	3.83985900	-1.56949700	-0.07097900
H	1.72955500	-1.89035600	0.00678600
C	4.57871300	0.72623600	-0.03475800
H	3.05259500	2.21406700	0.07594900
C	4.87478800	-0.63522800	-0.08731900
H	4.06591100	-2.62987300	-0.11205500
H	5.38069200	1.45687100	-0.04777600
H	5.90642600	-0.96627100	-0.14095100

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -635.476354616
E_0 = -635.183544
H = -635.166313
G = -635.229971

0 1

C	0.293136	0.622809	0.249815
C	1.182412	-0.541728	-0.272334
C	0.644860	1.967771	-0.430522
H	0.470020	1.924924	-1.511976
H	0.033877	2.788331	-0.039533
H	1.695313	2.248978	-0.285614
Be	-1.395976	0.347605	0.154112
C	-3.083162	0.134891	0.067000
C	-3.680102	-1.127243	-0.138025
C	-3.964875	1.229858	0.197357
C	-5.065152	-1.290945	-0.208492
H	-3.053905	-2.009162	-0.245921
C	-5.351530	1.079787	0.129165
H	-3.563607	2.227663	0.356419
C	-5.905456	-0.184771	-0.074559
H	-5.489375	-2.277273	-0.367150
H	-5.998871	1.944606	0.234056
H	-6.982066	-0.307215	-0.128166
C	0.821225	-1.885008	0.393777
H	0.918603	-1.823172	1.482156
H	-0.209060	-2.177966	0.167739
H	1.476107	-2.689060	0.045385
C	2.679012	-0.275139	-0.128200
C	3.514867	-0.252695	-1.250816
C	3.265113	-0.059988	1.127679
C	4.887751	-0.024927	-1.130865
H	3.084925	-0.415501	-2.234652
C	4.634463	0.166978	1.255638
H	2.645337	-0.065207	2.018377
C	5.454166	0.185690	0.125047
H	5.511507	-0.011474	-2.018397
H	5.063520	0.330445	2.238650
H	6.519317	0.363305	0.223872
H	0.509681	0.734644	1.326087
H	0.992215	-0.649329	-1.347757

Products (Ph-Be-Ph)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.249516985
E_0 = -633.979844
H = -633.962580
G = -634.027224

0 1

C	0.89681100	0.87067700	0.02447300
C	1.24807500	2.18003600	0.00917500
C	2.66595800	2.69587700	0.07198000
H	2.76953300	3.41333300	0.89454700
H	3.39724000	1.90116600	0.21153800
H	2.92091900	3.24144800	-0.84483000
Be	-0.71349800	0.41066300	-0.00652900
C	-2.32378200	-0.06145000	-0.03923400
C	-3.15826900	0.06783600	1.09123000
C	-2.91409100	-0.60755500	-1.19874600
C	-4.49678100	-0.32172200	1.06979900
H	-2.75936600	0.48134500	2.01420500
C	-4.25130300	-1.00064400	-1.23096500
H	-2.32061800	-0.73222500	-2.10086500
C	-5.04597300	-0.85757600	-0.09429100
H	-5.11058700	-0.20917700	1.95740000
H	-4.67385900	-1.41797100	-2.13901900
H	-6.08679600	-1.16248000	-0.11545300
C	1.91282300	-0.22521900	0.04714200
C	1.99320700	-1.10152100	1.14153200
C	2.76782600	-0.46140100	-1.04180600
C	2.90671500	-2.15356000	1.15971600
H	1.33834300	-0.94648800	1.99343300
C	3.67748200	-1.51696400	-1.02888500
H	2.71044700	0.18823300	-1.90875600
C	3.75366700	-2.36721600	0.07332400
H	2.95421900	-2.80902700	2.02267500
H	4.32624900	-1.67700900	-1.88351600
H	4.46041600	-3.18924600	0.08312800
C	0.21382500	3.28078000	-0.04840000
H	0.37358900	3.91907100	-0.92557200
H	-0.81066900	2.89995000	-0.09804700
H	0.28780600	3.93415900	0.82898400

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.245797515
E_0 = -633.976391
H = -633.958883
G = -634.024013

0 1

C	-0.879727	1.973933	0.079727
C	-2.073311	1.330313	0.016775
C	-0.804631	3.494861	0.033403
H	0.200450	3.859903	0.262461
H	-1.058701	3.882031	-0.960954
H	-1.485956	3.971135	0.747394
C	-3.413873	2.012370	-0.152748
H	-4.158222	1.596885	0.533483
H	-3.348753	3.086736	0.017224
H	-3.804892	1.869390	-1.167107
Be	0.522376	1.048450	0.063680
C	2.059218	0.369620	-0.035399
C	2.282688	-0.997952	-0.299269
C	3.207822	1.173206	0.129827
C	3.567319	-1.531242	-0.394571
H	1.435990	-1.665377	-0.433097
C	4.497425	0.649468	0.041026
H	3.101224	2.235967	0.334092
C	4.679153	-0.707127	-0.222947
H	3.703154	-2.587882	-0.601204
H	5.358048	1.296464	0.175894
H	5.680039	-1.119434	-0.294372
C	-2.108353	-0.159135	0.087629
C	-2.892315	-0.920968	-0.796486
C	-1.344245	-0.851138	1.042883
C	-2.878020	-2.311221	-0.753272
H	-3.501041	-0.420779	-1.540815
C	-1.326998	-2.245901	1.085325
H	-0.799892	-0.287691	1.793977
C	-2.091056	-2.982100	0.184640
H	-3.480036	-2.875565	-1.457163
H	-0.731501	-2.751929	1.837152
H	-2.085988	-4.065577	0.219052

Products (Ph-Be-Ph)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1019.02152621
E_0 = -1018.623125
H = -1018.599284
G = -1018.680117

0 1

Be	0.41749300	-0.70665000	0.07889800
C	-0.86828000	0.36603100	-0.32013800
C	-0.37658200	1.40920300	-1.36778200
H	-0.43895400	0.94023700	-2.35241500
C	-1.98440400	-0.46971400	-0.96744000
C	-3.34300500	-0.27870500	-0.67859400
C	-1.66015200	-1.43979000	-1.93116400
C	-4.33043800	-1.02360100	-1.32283700
H	-3.63466300	0.45982100	0.05816500
C	-2.64244800	-2.18641600	-2.57684500
H	-0.61797700	-1.61592800	-2.18742300
C	-3.98751400	-1.98223900	-2.27352400
H	-5.37337900	-0.84957500	-1.08015000
H	-2.35546200	-2.93094800	-3.31143800
H	-4.75624200	-2.56337800	-2.77016500
C	1.54134100	-1.89431600	0.45461800
C	1.12283100	-3.18917200	0.82963400
C	2.93313600	-1.67004200	0.40412300
C	2.03365900	-4.19752700	1.14128300
H	0.06237300	-3.42354000	0.87798700
C	3.85171000	-2.67299900	0.71110000
H	3.31067800	-0.69260600	0.11813100
C	3.40257100	-3.93970400	1.08221900
H	1.67852800	-5.18201600	1.42751000
H	4.91614400	-2.46832200	0.66169700
H	4.11490100	-4.72169300	1.32282700
C	-1.31017500	0.96635700	1.01450500
C	-1.39305800	2.34327000	1.26418600
C	-1.63704200	0.10372400	2.07882700
C	-1.78626000	2.83408400	2.51092200
H	-1.14378400	3.05434600	0.48668700
C	-2.02891700	0.58713900	3.32219200
H	-1.59989100	-0.97120000	1.92335100
C	-2.10643600	1.96209600	3.54666400
H	-1.83900200	3.90612100	2.66804000
H	-2.27176700	-0.10975800	4.11689100
H	-2.40790000	2.34465900	4.51509700
C	1.03905300	1.95005900	-1.22208700
C	1.69918400	2.43223500	-2.36256700
C	1.73090300	1.98588300	-0.00549700
C	2.99557500	2.93211800	-2.29218600
H	1.18710400	2.40839400	-3.31969300
C	3.03570800	2.48086600	0.06909600
H	1.24763600	1.65901000	0.90848900
C	3.67266600	2.95710200	-1.07197900
H	3.48177500	3.29547100	-3.19099400
H	3.54640700	2.49791100	1.02565100
H	4.68419900	3.34285400	-1.01488700
H	-1.08244700	2.25108800	-1.41933300

Products (Ph-Be-Ph)

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1019.028781160
E_0 = -1018.630331
H = -1018.606427
G = -1018.688480

0 1

Be	-1.513095	0.258640	0.256279
C	0.166418	0.462473	0.459937
C	1.019553	-0.512922	-0.395948
C	0.558527	-1.947950	-0.128568
C	-3.177647	0.206999	0.077397
C	-3.926171	1.383634	-0.141047
C	-3.902410	-1.001855	0.146436
C	-5.312952	1.357812	-0.282564
H	-3.419804	2.343209	-0.202971
C	-5.289147	-1.036660	0.007960
H	-3.375919	-1.938126	0.310288
C	-5.997095	0.145241	-0.207691
H	-5.859614	2.279861	-0.450390
H	-5.818123	-1.982180	0.067406
H	-7.076209	0.121392	-0.316270
C	0.949177	-2.640510	1.024219
C	-0.311656	-2.585636	-1.020472
C	0.476262	-3.925271	1.280441
H	1.642087	-2.177317	1.717906
C	-0.785653	-3.873789	-0.768725
H	-0.617204	-2.074090	-1.928604
C	-0.394446	-4.547588	0.385420
H	0.793897	-4.445116	2.177755
H	-1.454059	-4.349393	-1.478092
H	-0.757062	-5.549957	0.583262
H	0.798738	-0.323029	-1.451869
H	0.353425	0.240954	1.520490
C	0.397687	1.943777	0.243089
C	0.233375	2.841559	1.312486
C	0.699499	2.488776	-1.015378
C	0.364717	4.216334	1.136184
H	0.005079	2.451691	2.300571
C	0.835305	3.864358	-1.193321
H	0.843424	1.835649	-1.868623
C	0.667712	4.737856	-0.120803
H	0.236638	4.880435	1.984284
H	1.077183	4.253557	-2.176524
H	0.775207	5.807300	-0.260949
C	2.537350	-0.371347	-0.252763
C	3.358483	-0.837484	-1.287891
C	3.150151	0.178568	0.875780
C	4.745339	-0.764126	-1.198018
H	2.902829	-1.267542	-2.174927
C	4.540562	0.251705	0.972964
H	2.545164	0.571153	1.684046
C	5.343756	-0.219364	-0.061855
H	5.359036	-1.129588	-2.014221
H	4.993742	0.686806	1.857101
H	6.423741	-0.157757	0.011602

Products (Ph-Be-Ph)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1017.814839800
E_0 = -1017.439252
H = -1017.415796
G = -1017.495382

0 1

C	-0.181551	0.523303	0.100187
C	-0.930967	-0.615217	0.051451
Be	1.498872	0.375164	0.061862
C	3.169518	0.505083	-0.065021
C	4.012604	-0.593405	-0.334086
C	3.798126	1.760401	0.083394
C	5.394535	-0.451343	-0.450007
H	3.583945	-1.584350	-0.454448
C	5.180186	1.912192	-0.025605
H	3.199710	2.644068	0.290434
C	5.981891	0.803922	-0.294255
H	6.014295	-1.317106	-0.659630
H	5.631061	2.891505	0.097123
H	7.057269	0.917270	-0.381318
C	-0.229640	-1.930636	0.142552
C	-0.519247	-2.975352	-0.752200
C	0.768391	-2.145709	1.107313
C	0.191048	-4.169299	-0.707989
H	-1.296453	-2.836926	-1.494870
C	1.479291	-3.346719	1.154078
H	0.950796	-1.386158	1.860827
C	1.196620	-4.359699	0.243448
H	-0.036785	-4.955765	-1.419062
H	2.239173	-3.491349	1.913894
H	1.743136	-5.295276	0.279419
C	-2.412285	-0.674966	-0.126578
C	-3.061444	0.088180	-1.108160
C	-3.189648	-1.525682	0.674775
C	-4.441423	0.011596	-1.274756
H	-2.477848	0.740146	-1.746326
C	-4.571851	-1.590693	0.519523
H	-2.706164	-2.134977	1.430341
C	-5.203396	-0.822918	-0.457813
H	-4.922435	0.604614	-2.044779
H	-5.154892	-2.244803	1.158547
H	-6.278656	-0.878660	-0.585657
C	-0.762263	1.891324	0.164509
C	-0.297732	2.898163	-0.699205
C	-1.716278	2.249796	1.132481
C	-0.789273	4.199623	-0.623661
H	0.446044	2.651830	-1.451398
C	-2.196749	3.552896	1.218969
H	-2.077143	1.497098	1.823733
C	-1.741485	4.533906	0.337595
H	-0.423657	4.953326	-1.312679
H	-2.929936	3.804342	1.977824
H	-2.118825	5.548036	0.404943

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1017.814839800
E_0 = -1017.439252
H = -1017.415796
G = -1017.495382

0 1

C	-0.181551	0.523303	0.100187
C	-0.930967	-0.615217	0.051451
Be	1.498872	0.375164	0.061862
C	3.169518	0.505083	-0.065021
C	4.012604	-0.593405	-0.334086
C	3.798126	1.760401	0.083394
C	5.394535	-0.451343	-0.450007
H	3.583945	-1.584350	-0.454448
C	5.180186	1.912192	-0.025605
H	3.199710	2.644068	0.290434
C	5.981891	0.803922	-0.294255
H	6.014295	-1.317106	-0.659630
H	5.631061	2.891505	0.097123
H	7.057269	0.917270	-0.381318
C	-0.229640	-1.930636	0.142552
C	-0.519247	-2.975352	-0.752200
C	0.768391	-2.145709	1.107313
C	0.191048	-4.169299	-0.707989
H	-1.296453	-2.836926	-1.494870
C	1.479291	-3.346719	1.154078
H	0.950796	-1.386158	1.860827
C	1.196620	-4.359699	0.243448
H	-0.036785	-4.955765	-1.419062
H	2.239173	-3.491349	1.913894
H	1.743136	-5.295276	0.279419
C	-2.412285	-0.674966	-0.126578
C	-3.061444	0.088180	-1.108160
C	-3.189648	-1.525682	0.674775
C	-4.441423	0.011596	-1.274756
H	-2.477848	0.740146	-1.746326
C	-4.571851	-1.590693	0.519523
H	-2.706164	-2.134977	1.430341
C	-5.203396	-0.822918	-0.457813
H	-4.922435	0.604614	-2.044779
H	-5.154892	-2.244803	1.158547
H	-6.278656	-0.878660	-0.585657
C	-0.762263	1.891324	0.164509
C	-0.297732	2.898163	-0.699205
C	-1.716278	2.249796	1.132481
C	-0.789273	4.199623	-0.623661
H	0.446044	2.651830	-1.451398
C	-2.196749	3.552896	1.218969
H	-2.077143	1.497098	1.823733
C	-1.741485	4.533906	0.337595
H	-0.423657	4.953326	-1.312679
H	-2.929936	3.804342	1.977824
H	-2.118825	5.548036	0.404943

Products (Ph-Be-Ph)

(1,1)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -786.704853104
E_0 = -786.409396
H = -786.390695
G = -786.460492

0 1

C	0.04221900	-0.05969100	0.01791300
C	0.77065100	-1.20557100	-0.01565600
Be	-1.62415200	-0.23574500	0.00812900
C	-3.28480700	-0.46221600	-0.00674100
C	-3.97169100	-0.99107800	1.10671100
C	-4.06771100	-0.13362300	-1.13393300
C	-5.35276200	-1.18160300	1.09881400
H	-3.42111100	-1.26216600	2.00393700
C	-5.44921200	-0.31925800	-1.15147400
H	-3.59363300	0.27795900	-2.02121800
C	-6.09442800	-0.84482100	-0.03272400
H	-5.85051300	-1.59087100	1.97167200
H	-6.02230400	-0.05528200	-2.03409400
H	-7.16924900	-0.99087700	-0.04264300
C	2.22636100	-1.44539400	0.02682700
C	3.16003000	-0.53682800	0.55579200
C	2.70512200	-2.67978900	-0.44684800
C	4.51516700	-0.84862000	0.58752100
H	2.82349200	0.40981800	0.95496400
C	4.06207700	-2.98598900	-0.42752800
H	1.99812700	-3.40374300	-0.83979400
C	4.97483100	-2.06844500	0.08974700
H	5.21722200	-0.13617400	1.00658600
H	4.40555300	-3.94150300	-0.80814700
H	6.03284300	-2.30416800	0.11383800
C	0.62336600	1.31260800	0.00016300
C	0.38894500	2.20516000	1.05800800
C	1.34361700	1.78246200	-1.11050200
C	0.88370200	3.50781400	1.02339600
H	-0.17476400	1.86866600	1.92259500
C	1.82787700	3.08706000	-1.15057500
H	1.52299700	1.11374800	-1.94504700
C	1.60533400	3.95547100	-0.08167200
H	0.69926700	4.17453800	1.85879400
H	2.38103300	3.42717600	-2.01947200
H	1.98338400	4.97100800	-0.11356100
H	0.21213400	-2.14103800	-0.08436500

(1,2)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -786.708430522
E_0 = -786.413069
H = -786.394542
G = -786.462332

0 1

C	-0.23686600	-1.40625300	-0.19484800
C	-1.19927400	-0.45298600	-0.10599600
Be	1.40331500	-1.10011100	-0.12683000
C	3.07375100	-0.95658100	-0.02658700
C	3.71117200	0.25746300	0.30564200
C	3.91452600	-2.06542900	-0.26212100
C	5.09837500	0.36093700	0.39836400
H	3.11422900	1.14517300	0.49621700
C	5.30310500	-1.97203800	-0.17453100
H	3.48184500	-3.02868600	-0.52133000
C	5.89807300	-0.75566100	0.15702700
H	5.55655500	1.30986700	0.65731300
H	5.92009600	-2.84441800	-0.36326200
H	6.97786000	-0.67836000	0.22687900
C	-0.81394100	0.99010600	-0.06286700
C	-1.34087200	1.85238300	0.91217400
C	0.11919600	1.51069500	-0.97232200
C	-0.92081900	3.17592500	0.99567100
H	-2.07123500	1.47312400	1.61783300
C	0.53528700	2.84000700	-0.89379200
H	0.49179800	0.87689300	-1.77021500
C	0.02052000	3.67559600	0.09383100
H	-1.32733300	3.82045800	1.76730100
H	1.25071300	3.22229600	-1.61344600
H	0.34021400	4.70965700	0.15609500
C	-2.65362300	-0.77291300	-0.04605500
C	-3.11763800	-1.90895300	0.63569000
C	-3.59743200	0.04027400	-0.69374800
C	-4.47182700	-2.22930200	0.65572000
H	-2.40972200	-2.53228000	1.16948700
C	-4.95106400	-0.28567200	-0.68369000
H	-3.26453400	0.92593900	-1.22231800
C	-5.39468100	-1.42119600	-0.00779500
H	-4.80874100	-3.10624500	1.19757600
H	-5.66022900	0.34881100	-1.20382900
H	-6.44973100	-1.67045700	0.00801700
H	-0.61084000	-2.42974800	-0.27359800

Products ($B(C_6F_5)_3$)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2364.99111384
E_0 = -2364.750051
H = -2364.714534
G = -2364.819020

0 1

C	0.42644300	-1.20472400	1.89585200
C	-0.69727000	-1.93941400	1.73167900
C	1.35577600	-1.47304700	3.07445000
H	2.20366900	-0.78617500	3.08235800
H	0.82718200	-1.33458600	4.02161700
H	1.75615800	-2.49014500	3.05582900
C	-1.11583500	-3.06936000	2.64068000
H	-1.03903600	-4.02824100	2.11508600
H	-0.50825500	-3.12667900	3.54164800
H	-2.16186400	-2.95408000	2.93953500
C	-1.60681700	-1.76064300	0.55374900
C	-2.90501000	-1.26882700	0.71038400
C	-1.24661600	-2.15656800	-0.73543400
C	-3.79026900	-1.14669200	-0.35126800
C	-2.11517700	-2.05329900	-1.81704600
C	-3.39199000	-1.54269000	-1.62424000
B	0.84800300	-0.07654100	0.90670000
C	2.32622400	0.01034700	0.36816600
C	3.10800900	-1.13468600	0.15024600
C	2.95195100	1.22587800	0.05254700
C	4.39693800	-1.08756900	-0.36267000
C	4.24454200	1.31080500	-0.44358300
C	4.96871000	0.14388600	-0.65941500
C	-0.18787900	1.04225500	0.49196400
C	-0.42075100	1.41285900	-0.83305900
C	-0.91762900	1.73981500	1.45665900
C	-1.33368800	2.39230900	-1.19458300
C	-1.82358600	2.74250700	1.13618600
C	-2.03592300	3.06511500	-0.19926500
F	-0.72042700	1.48297600	2.76174300
F	-2.48511300	3.40019000	2.09185800
F	-2.90918500	4.01584700	-0.52602100
F	-1.54478600	2.69615500	-2.47843000
F	0.23532700	0.78002100	-1.82501600
F	2.31587100	2.39127400	0.25590600
F	2.61861400	-2.35236600	0.41813000
F	5.09340500	-2.20850100	-0.56815200
F	6.20642400	0.20656800	-1.14091900
F	4.79963700	2.49519800	-0.71257400
F	-0.02909700	-2.67159100	-0.96595300
F	-1.73113300	-2.44390900	-3.03463400
F	-4.23268600	-1.43122000	-2.65239700
F	-5.01477600	-0.64639400	-0.16319600
F	-3.31971700	-0.86834800	1.92392600

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2364.98882883
E_0 = -2364.747817
H = -2364.712399
G = -2364.816812

0 1

C	0.85108800	0.33190200	1.33421400
C	0.84225600	0.63660800	2.64811900
C	2.07545000	0.93185500	3.45977700
H	2.08760000	0.31462600	4.36400600
H	3.00158800	0.75401200	2.91462800
H	2.06898400	1.97707700	3.78915400
C	2.12046700	0.34367300	0.53788600
C	2.66513900	-0.79917900	-0.05439000
C	2.82064800	1.53611600	0.31386900
C	3.81838900	-0.76995300	-0.82895000
C	3.97687200	1.59379800	-0.45345300
C	4.47743900	0.43476700	-1.03369700
C	-0.43290100	0.65699100	3.45174800
H	-0.55132700	1.62161300	3.95737000
H	-1.32931800	0.47401500	2.85716100
H	-0.39866800	-0.10949700	4.23316200
B	-0.47269300	0.00110100	0.53866800
C	-1.46251700	1.16446400	0.12291100
C	-1.04177100	2.30323500	-0.56569900
C	-2.82458000	1.11051400	0.42673000
C	-1.90531300	3.32522500	-0.93506100
C	-3.71473700	2.12295700	0.09850500
C	-3.25001700	3.23648500	-0.59263300
C	-0.85878600	-1.46426100	0.11654800
C	-1.38060700	-1.75230300	-1.15054100
C	-0.71020900	-2.56270800	0.97220800
C	-1.71468700	-3.03535300	-1.55871000
C	-1.05954500	-3.85438100	0.60737900
C	-1.55769400	-4.09199900	-0.66906600
F	-3.31558800	0.05543000	1.10738500
F	-5.00406800	2.04031200	0.43817200
F	-4.09043800	4.21369500	-0.92613400
F	-1.46159000	4.38382800	-1.61703800
F	0.24056400	2.41359600	-0.95020900
F	-1.53893400	-0.76859100	-2.05409200
F	-2.18316700	-3.26481400	-2.78811100
F	-1.88417600	-5.32749000	-1.03742600
F	-0.25171200	-2.39044500	2.22012000
F	-0.92274300	-4.86921500	1.46464600
F	2.08889700	-1.99862800	0.13960500
F	4.30229500	-1.89493300	-1.36525300
F	5.58695500	0.47758200	-1.77231600
F	2.38742100	2.68189100	0.85763400
F	4.61054200	2.75577700	-0.63864600

Products ($B(C_6F_5)_3$)

(1,1)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2517.45370310
E_0 = -2517.187075
H = -2517.150318
G = -2517.258069

0 1

C	0.35697200	-1.32794000	-0.23765600
C	-0.26643300	-2.41013600	-0.77012000
C	1.74705400	-1.49534200	0.27174800
C	2.73310500	-2.23695200	-0.39376600
C	2.15224100	-0.88537200	1.46397300
C	4.02604300	-2.36801700	0.09847100
C	3.43364900	-1.00275100	1.98152700
C	4.37943700	-1.75269700	1.29305800
B	-0.30542500	0.08300600	-0.08217900
C	-1.76903600	0.22773900	0.48684200
C	-2.24297800	-0.55576700	1.54533400
C	-2.67650900	1.16492800	-0.01739900
C	-3.52073700	-0.41743000	2.07250100
C	-3.96491600	1.31684600	0.46897500
C	-4.38763500	0.52150400	1.52854900
C	0.52259300	1.38109900	-0.43060600
C	0.45707500	2.55308100	0.33329200
C	1.38654800	1.43117900	-1.53095800
C	1.19835600	3.68922000	0.04187800
C	2.12834800	2.55577400	-1.86474200
C	2.03506000	3.69125700	-1.06873300
F	-2.32363400	1.94594600	-1.05631200
F	-4.80203200	2.21001600	-0.06798600
F	-5.61999000	0.65600900	2.01466400
F	-3.92373700	-1.17875600	3.09453300
F	-1.45400100	-1.47305100	2.12543000
F	-0.32739800	2.60883200	1.42079600
F	1.11557000	4.77770000	0.81105000
F	2.74491900	4.77613900	-1.36746700
F	1.50543800	0.36656800	-2.34359500
F	2.92491700	2.55903600	-2.93730200
F	2.46522900	-2.83445200	-1.56472000
F	4.93574400	-3.07789200	-0.57523000
F	5.61662400	-1.87822600	1.77341300
F	1.26457800	-0.14997400	2.16039900
F	3.76052600	-0.40783300	3.13209700
C	-1.54366100	-2.42667000	-1.48310500
C	-2.39769400	-3.53640500	-1.34866300
C	-1.93080900	-1.38459600	-2.34210600
C	-3.62528100	-3.56933600	-1.99822600
H	-2.09977900	-4.36305900	-0.71243000
C	-3.15643600	-1.42352500	-3.00068100
H	-1.24339500	-0.56913700	-2.53667100
C	-4.01084400	-2.51005700	-2.82283400
H	-4.28037800	-4.42334800	-1.86976200
H	-3.43486500	-0.61543100	-3.66734200
H	-4.96230300	-2.54379000	-3.34106700
H	0.22200400	-3.37862800	-0.69909300

(1,2)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2517.45287749
E_0 = -2517.186197
H = -2517.149385
G = -2517.258145

0 1

C	0.19559600	1.59047900	-0.45650100
C	-1.12948500	1.78521100	-0.22617500
C	-2.01492900	0.71997700	0.33293200
C	-3.15409600	0.29801000	-0.36013400
C	-1.79004200	0.13804300	1.58236800
C	-4.01413800	-0.66686800	0.14695500
C	-2.64356700	-0.81980300	2.11725500
C	-3.75796300	-1.22688700	1.39389100
B	1.06347400	0.32525200	-0.33567100
C	2.61771300	0.51148600	-0.12914100
C	3.14384000	1.53227600	0.67397600
C	3.56787000	-0.32140200	-0.73439400
C	4.50515800	1.71230000	0.87738100
C	4.93595700	-0.15879900	-0.57025900
C	5.40655700	0.86244000	0.24715700
C	0.50484000	-1.14716400	-0.47800900
C	0.82619900	-2.15038900	0.43884300
C	-0.28360200	-1.54505600	-1.55939400
C	0.38276200	-3.45969900	0.31555300
C	-0.72892500	-2.84943900	-1.72871400
C	-0.39725200	-3.81097300	-0.78079700
F	-0.61321200	-0.65736400	-2.51417700
F	-1.46883900	-3.18927600	-2.78826400
F	-0.82580500	-5.06412700	-0.92197200
F	0.69875900	-4.38143300	1.22939000
F	1.58339700	-1.85607600	1.51146900
F	3.17576300	-1.31643000	-1.54925400
F	2.32339900	2.37596300	1.31947500
F	4.95685800	2.68912000	1.66882600
F	6.71515900	1.02775800	0.42249800
F	5.80201200	-0.96681700	-1.18798100
F	-0.73605800	0.50997800	2.32284100
F	-2.40078700	-1.34885900	3.31909600
F	-4.57748700	-2.15124300	1.89202000
F	-5.08123700	-1.06119400	-0.55135400
F	-3.43037800	0.81121800	-1.56415600
C	-1.77247200	3.10161000	-0.45682500
C	-1.36280700	3.92269500	-1.52053600
C	-2.79629900	3.56153100	0.38635500
C	-1.95018400	5.16524300	-1.72474800
H	-0.60474900	3.56849700	-2.20872200
C	-3.37331800	4.81213600	0.18926100
H	-3.12826300	2.94808600	1.21588600
C	-2.95350500	5.61769900	-0.86724500
H	-1.63269600	5.77827700	-2.56046200
H	-4.15113700	5.15681600	0.86083700
H	-3.40979500	6.58779600	-1.02729500
H	0.73192900	2.49537400	-0.73233400

Adduct ($B(C_6F_5)_3$)

(1,1)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2517.39133405
E_0 = -2517.127851
H = -2517.090621
G = -2517.198459

0 1

C	-1.460001	0.082024	2.154326
C	-0.237165	0.106754	1.896442
C	-0.806432	-0.413916	-0.801410
C	-1.581522	-1.550435	-0.559071
C	-1.137308	0.255108	-1.980927
C	-2.621168	-1.977236	-1.370991
C	-2.169301	-0.139020	-2.828539
C	-2.923706	-1.260074	-2.520355
C	1.596950	-1.111330	0.317969
C	1.777150	-2.150707	-0.601165
C	2.548620	-1.104270	1.343817
C	2.778038	-3.111666	-0.497539
C	3.556637	-2.044233	1.492176
C	3.672234	-3.066394	0.560671
B	0.410829	0.018366	0.205366
C	0.942591	1.555633	0.005133
C	2.251333	1.906224	-0.338597
C	0.087080	2.650468	0.162001
C	2.684545	3.220545	-0.487199
C	0.477099	3.974380	0.031785
C	1.794595	4.265842	-0.293790
F	-0.441097	1.335301	-2.388164
F	-2.436747	0.555903	-3.941028
F	-3.922074	-1.649153	-3.318322
F	-3.326922	-3.075332	-1.061954
F	-1.313199	-2.332080	0.515875
F	3.184801	0.965310	-0.580827
F	3.953527	3.482942	-0.820410
F	2.193743	5.532228	-0.429575
F	-0.405796	4.968456	0.202327
F	-1.227577	2.452280	0.426039
F	2.546650	-0.108576	2.268006
F	4.423814	-1.964600	2.508928
F	4.636905	-3.981103	0.674911
F	2.888030	-4.077259	-1.417388
F	0.988313	-2.267675	-1.687762
C	-2.840505	0.047710	2.331098
C	-3.492854	-1.181664	2.599534
C	-3.594474	1.245590	2.256136
C	-4.864092	-1.203356	2.788344
H	-2.906541	-2.090374	2.641284
C	-4.965312	1.205111	2.446712
H	-3.084261	2.174973	2.039620
C	-5.596196	-0.014250	2.712033
H	-5.369103	-2.140119	2.989629
H	-5.548134	2.116130	2.386747
H	-6.670398	-0.038838	2.857655
H	0.581932	0.235597	2.590760

Products ($Be(C_6F_5)_2$)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1626.88072230
E_0 = -1626.692284
H = -1626.666072
G = -1626.751258

0 1

C	-0.985966	1.452218	-0.088645
C	-1.200732	2.790846	-0.150961
Be	0.575418	0.865720	-0.094128
C	2.145249	0.241143	-0.136422
C	2.454254	-0.894236	-0.877494
C	3.199824	0.810204	0.568494
C	3.726711	-1.446054	-0.929987
F	1.476898	-1.502780	-1.586275
C	4.490476	0.300065	0.550180
F	2.974870	1.917544	1.311432
C	4.749586	-0.838799	-0.207097
F	3.984692	-2.539396	-1.654610
F	5.479403	0.876952	1.240948
F	5.980396	-1.348606	-0.240551
C	-2.100080	0.479991	0.070899
C	-2.057465	-0.481865	1.085750
C	-3.184390	0.381371	-0.807481
C	-3.031075	-1.454925	1.253933
F	-1.014643	-0.477248	1.943834
C	-4.174659	-0.584438	-0.668835
F	-3.284677	1.224213	-1.849452
C	-4.102549	-1.504621	0.369403
F	-2.948160	-2.339837	2.252652
F	-5.193921	-0.638209	-1.533139
F	-5.051258	-2.432606	0.513878
C	-0.057991	3.752896	-0.367651
H	-0.234228	4.360064	-1.262701
H	0.031761	4.449006	0.473154
H	0.908317	3.254792	-0.494438
C	-2.537852	3.467626	-0.000779
H	-2.451685	4.326190	0.672842
H	-2.879156	3.855773	-0.967091
H	-3.309153	2.802510	0.386454

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1626.87199276
E_0 = -1626.683880
H = -1626.657384
G = -1626.742960

0 1

C	-0.937274	2.738258	-0.368408
C	-2.166976	2.208623	-0.181167
Be	0.365636	1.688856	-0.320808
C	1.737748	0.700520	-0.281283
C	1.729843	-0.629747	-0.685086
C	2.958996	1.186706	0.173111
C	2.853267	-1.443883	-0.648610
F	0.578003	-1.175958	-1.137880
C	4.112612	0.417263	0.230005
F	3.043118	2.473471	0.581072
C	4.052506	-0.909822	-0.185580
F	2.804008	-2.719152	-1.046053
F	5.268334	0.922781	0.672453
F	5.145498	-1.670591	-0.140668
C	-2.289356	0.729777	0.074778
C	-2.760691	-0.143435	-0.908964
C	-1.987337	0.161433	1.314187
C	-2.906015	-1.506298	-0.690207
F	-3.074432	0.335476	-2.123597
C	-2.122624	-1.200827	1.561654
F	-1.560135	0.937177	2.325423
C	-2.583258	-2.037544	0.553847
F	-3.341160	-2.310935	-1.663351
F	-1.817336	-1.707276	2.760409
F	-2.711493	-3.345661	0.775913
C	-0.704493	4.215565	-0.623824
H	-1.610318	4.824114	-0.591147
H	-0.006166	4.628068	0.112487
H	-0.241433	4.368965	-1.605052
C	-3.496607	2.925804	-0.186830
H	-3.398741	3.989782	-0.395197
H	-4.163082	2.492974	-0.939701
H	-3.994493	2.812324	0.782622

Products ($Be(C_6F_5)_2$)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2010.44673885
E_0 = -2010.152529
H = -2010.120032
G = -2010.219723

0 1

Be	0.922891	0.071375	0.168146
C	-1.647968	-0.970842	0.159991
C	-1.357951	-2.091003	-0.626498
C	-2.754964	-1.097851	1.008739
C	-2.123940	-3.247179	-0.614620
C	-3.535898	-2.245877	1.048508
C	-3.225359	-3.324847	0.229550
C	2.572592	-0.304944	0.060035
C	3.346435	-0.565083	1.184070
C	3.235754	-0.376072	-1.159601
C	4.696387	-0.881890	1.125909
C	4.584003	-0.687874	-1.274847
C	5.315615	-0.942056	-0.118896
C	-1.192789	1.489443	0.015422
C	-0.748853	0.204761	0.152487
C	-2.571983	1.901233	-0.359083
C	-3.217092	2.939382	0.329981
C	-3.248770	1.278556	-1.418124
C	-4.511929	3.319910	-0.008339
H	-2.706508	3.437288	1.146372
C	-4.538200	1.671112	-1.766922
H	-2.752851	0.499041	-1.984222
C	-5.176802	2.687537	-1.058389
H	-5.001867	4.111936	0.546686
H	-5.041637	1.186879	-2.596126
H	-6.182780	2.989563	-1.326687
C	-0.188697	2.575102	0.205765
C	-0.085821	3.646160	-0.698878
C	0.723364	2.514133	1.274596
C	0.920822	4.593505	-0.561269
H	-0.786832	3.716497	-1.522231
C	1.731188	3.471888	1.413063
H	0.595991	1.756247	2.041345
C	1.836312	4.507653	0.491989
H	0.998005	5.402003	-1.279483
H	2.415574	3.413327	2.251596
H	2.614909	5.254365	0.597215
F	2.769931	-0.509097	2.408925
F	5.406357	-1.125520	2.234207
F	2.553422	-0.128124	-2.298722
F	5.187987	-0.744381	-2.467379
F	6.612685	-1.242425	-0.203812
F	-0.287725	-2.051874	-1.447168
F	-1.812605	-4.281201	-1.403789
F	-3.974276	-4.430107	0.258878
F	-4.582989	-2.323753	1.877351
F	-3.079045	-0.101495	1.846522

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2010.43801096
E_0 = -2010.143999
H = -2010.111374
G = -2010.212448

0 1

C	-1.079397	1.115187	-0.093135
C	-1.835139	-0.008669	0.012056
Be	0.591825	1.012728	-0.113961
C	2.278738	0.940071	-0.162320
C	2.954313	-0.103125	-0.786041
C	3.078696	1.919615	0.416981
C	4.338072	-0.188890	-0.843458
F	2.240972	-1.094687	-1.368772
C	4.466066	1.882696	0.387481
F	2.493233	2.963489	1.041716
C	5.095228	0.817207	-0.249961
F	4.950116	-1.209297	-1.452975
F	5.201877	2.843824	0.954856
F	6.425853	0.759715	-0.291826
C	-1.128020	-1.326582	0.163676
C	-1.161812	-2.286754	-0.852458
C	-0.418883	-1.667588	1.317547
C	-0.518186	-3.510816	-0.739506
F	-1.812686	-2.021995	-1.992506
C	0.230903	-2.889793	1.458399
F	-0.365134	-0.814748	2.356739
C	0.182241	-3.813734	0.423739
F	-0.553573	-4.394072	-1.740372
F	0.894248	-3.180239	2.581997
F	0.807894	-4.984783	0.541311
C	-3.322064	-0.095192	-0.023336
C	-4.071788	0.640088	-0.953732
C	-4.003580	-0.947341	0.858839
C	-5.457894	0.533896	-0.990493
H	-3.563785	1.284652	-1.659219
C	-5.392479	-1.040934	0.831924
H	-3.445814	-1.531161	1.582801
C	-6.124850	-0.300967	-0.094152
H	-6.019004	1.101513	-1.724247
H	-5.900861	-1.695163	1.531176
H	-7.205650	-0.379983	-0.123099
C	-1.646324	2.493847	-0.124216
C	-1.291785	3.379197	-1.154520
C	-2.463271	2.975266	0.911450
C	-1.766128	4.689229	-1.170780
H	-0.655973	3.031471	-1.963688
C	-2.925054	4.287794	0.902172
H	-2.730048	2.314683	1.728116
C	-2.584594	5.148956	-0.141216
H	-1.490623	5.350994	-1.984373
H	-3.552000	4.640621	1.713630
H	-2.946780	6.170614	-0.146401

Transition States (Me-Be-Me)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -250.571970989
E_0 = -250.417376
H = -250.404444
G = -250.456485

0 1			
C	-1.50053400	0.25675500	-0.02688000
C	-0.26631200	0.08154700	0.01616800
C	-2.88328400	0.72219300	-0.08556700
H	-3.43490900	0.46709300	0.82292700
H	-2.86024100	1.81133400	-0.17571700
H	-3.41135300	0.31777200	-0.95291200
Be	1.56315100	0.20671500	-0.00908400
C	2.05356100	1.87306700	0.06347900
H	1.78373000	2.33555000	1.02595000
H	1.57939800	2.50301000	-0.70424000
C	2.38272500	-1.32261200	-0.10730800
H	3.47486800	-1.22491600	-0.12103600
H	2.11883300	-1.88979800	-1.01565300
C	-1.03484900	-1.53207700	0.13917000
H	-0.48631800	-2.01817800	-0.66107600
H	-0.71110600	-1.85226900	1.12391400
H	-2.09814200	-1.75430800	0.01688500
H	2.14748100	-1.99714700	0.73221000
H	3.13731900	2.00176600	-0.04928700

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -250.616113396
E_0 = -250.457372
H = -250.445916
G = -250.492714

0 1			
C	-0.37333500	0.92089800	0.09849400
C	-0.87414500	-0.24248700	0.01407100
C	-0.74600900	2.36144500	0.06503300
H	-1.81594100	2.52281400	-0.10279900
H	-0.18724200	2.87798200	-0.71959700
H	-0.46868000	2.84068800	1.00794900
C	-2.09380100	-1.06407700	-0.17406300
H	-2.35544800	-1.61939600	0.73022600
H	-1.98498700	-1.78059200	-0.99110400
H	-2.92076100	-0.38786300	-0.41247700
Be	0.99568800	-0.10903300	0.04105000
C	2.67492300	0.22752800	-0.15485500
H	2.88839300	1.16236500	-0.68521900
H	3.15216800	0.32096900	0.83217600
C	0.52270400	-1.89319200	0.18332900
H	-0.26560100	-2.41773900	0.71306300
H	1.44622300	-2.03605600	0.75679700
H	0.65729000	-2.33085800	-0.80820700
H	3.20980600	-0.57686800	-0.67706200

Transition States (Me-Be-Me)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.148882793
E_0 = -633.887789
H = -633.869247
G = -633.936945

0 1

C	-0.29433600	-0.69958200	0.08021600
C	0.89214600	-1.12711600	0.07640000
Be	2.41058200	-2.15410900	0.14517600
C	2.83192100	-2.79285000	-1.41820600
H	3.79495200	-3.31905300	-1.40720700
H	2.89761200	-2.03023000	-2.20832100
C	3.06803200	-2.27473300	1.75138000
H	2.42673400	-2.89898700	2.39278100
H	3.16537400	-1.31510500	2.27983600
C	-1.70330600	-0.44609600	0.06373500
C	-2.25100800	0.79069500	0.43800000
C	-2.55729500	-1.49704900	-0.31918900
C	-3.62991700	0.96850600	0.43134900
H	-1.59474400	1.60303200	0.72368700
C	-3.93413800	-1.30972600	-0.30542900
H	-2.13452700	-2.44828600	-0.61852500
C	-4.47490800	-0.07864200	0.06581300
H	-4.04571600	1.92809300	0.71594900
H	-4.58604400	-2.12572300	-0.59490000
H	-5.54913600	0.06464800	0.06617100
C	1.79806200	2.53721500	0.98186300
C	1.94173600	3.11439800	-0.28162000
C	1.64125300	2.38155400	-1.43184800
C	1.19547300	1.07016900	-1.32464800
C	1.05078100	0.48480400	-0.05472000
C	1.34856900	1.22777900	1.10140800
H	2.03888400	3.10765400	1.87129400
H	2.29207200	4.13645400	-0.37021600
H	1.75889700	2.83233700	-2.41028600
H	0.96798300	0.48401400	-2.20642500
H	1.24234700	0.75912600	2.07188500
H	2.08269000	-3.51715200	-1.77311300
H	4.06191200	-2.74034700	1.75967100

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.183252537
E_0 = -633.918487
H = -633.901045
G = -633.964907

0 1

C	0.71720500	0.73086300	-0.18459900
C	-0.55998500	0.75855100	-0.15965800
Be	0.34059400	2.40628300	-0.12220300
C	-1.43864300	2.74256600	-0.48912300
H	-2.21002000	2.20666900	-1.02931000
H	-1.08253200	3.55772900	-1.13266200
C	1.32609600	3.78044100	0.21719300
H	2.08790100	3.59562600	0.98366300
H	0.74180300	4.65167800	0.54030700
C	-1.80289300	0.00284500	-0.05869400
C	-2.65291000	0.13221900	1.04914300
C	-2.12635800	-0.92086200	-1.06378400
C	-3.79610400	-0.65344800	1.15186300
H	-2.40821100	0.84373100	1.82886000
C	-3.27437000	-1.70202700	-0.95775800
H	-1.47519000	-1.01956300	-1.92452700
C	-4.11144600	-1.57069200	0.14884600
H	-4.44204200	-0.55089600	2.01648200
H	-3.51534800	-2.41148100	-1.74139000
H	-5.00499700	-2.17900000	0.23031800
C	1.83805800	-0.19158400	-0.05340300
C	3.15285400	0.29720300	-0.08417700
C	1.63684700	-1.57485900	0.10193900
C	4.23602700	-0.56902700	0.03708000
H	3.31089000	1.36252800	-0.20109100
C	2.72013400	-2.43833700	0.22274000
H	0.62650000	-1.96621600	0.12917700
C	4.02293000	-1.93804200	0.19032200
H	5.24616900	-0.17584500	0.01231900
H	2.55036400	-3.50261800	0.34327000
H	4.86632100	-2.61303600	0.28433100
H	1.87148200	4.09120800	-0.68579900
H	-1.85012100	3.16949200	0.42729000

Transition States (Et-Be-Et)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -330.443516349
E_0 = -330.209909
H = -330.194727
G = -330.251996

0 1

C	-2.40715600	0.25440300	0.37471500
C	-1.42201000	-0.29859100	-0.44204500
H	-3.45744100	-0.02611400	0.22232800
H	-1.74228800	0.87267000	-0.69208400
C	-2.14618200	1.16962600	1.53226100
H	-2.85565600	2.00017300	1.56425500
H	-2.29040900	0.58710700	2.44975600
H	-1.12424000	1.54999600	1.53093100
C	-1.88541100	-1.27320300	-1.50053400
H	-1.59490200	-2.27360200	-1.16562400
H	-2.96904700	-1.27344600	-1.67130600
H	-1.37389900	-1.10646300	-2.45117300
Be	0.38981500	-0.07877100	-0.19674600
C	1.02655200	-1.52390800	0.57371900
C	2.55008900	-1.61835900	0.78855800
H	0.69462300	-2.41481900	0.01422400
H	0.52455600	-1.63201100	1.55165300
H	2.85605400	-2.54276300	1.29736800
H	3.09153800	-1.58407900	-0.16297200
H	2.92463300	-0.78272700	1.38862400
C	1.04704700	1.43771300	-0.77510600
C	2.52000100	1.78644000	-0.48241300
H	0.41766000	2.28189700	-0.43696500
H	0.90054100	1.44389800	-1.87144200
H	2.83525600	2.74315800	-0.91995000
H	2.71036800	1.84972700	0.59477400
H	3.19581000	1.01775500	-0.87035500

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -330.483404072
E_0 = -330.243579
H = -330.229662
G = -330.282154

0 1

C	-1.364754	0.960695	-0.273193
C	-1.451070	-0.482140	-0.194090
H	-1.601548	1.365881	-1.257220
H	-1.883468	-0.887418	0.718650
C	-1.862386	1.805325	0.896783
H	-1.499081	2.833747	0.822482
H	-2.959144	1.847827	0.946345
H	-1.514208	1.417545	1.859944
C	-1.827832	-1.246961	-1.446613
H	-2.890771	-1.074284	-1.646747
H	-1.273092	-0.886425	-2.317217
H	-1.666186	-2.322964	-1.358934
Be	0.290488	0.421059	-0.231650
C	1.822826	1.137560	-0.574547
C	3.100911	0.279684	-0.612987
H	1.966749	1.961953	0.142037
H	1.715124	1.657132	-1.539773
H	4.000506	0.868427	-0.829349
H	3.283789	-0.232124	0.339159
H	3.045492	-0.499362	-1.382815
C	0.313096	-1.407726	0.358846
C	0.720265	-1.145380	1.815501
H	1.335785	-1.964648	2.202890
H	-0.158580	-1.065608	2.462792
H	1.303642	-0.227330	1.939525
H	-0.256282	-2.330434	0.298261
H	1.182973	-1.552497	-0.291635

Transition States (Et-Be-Et)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -329.208304642
E_0 = -328.996148
H = -328.980719
G = -329.039854

0 1

C	2.08340700	-0.29588900	-0.01455300
C	0.83646800	-0.27993600	0.00918500
C	3.52027900	-0.03620500	-0.04230200
H	3.99346400	-0.47096400	-0.92649500
H	3.65799900	1.04743000	-0.07695000
H	4.01653900	-0.41602300	0.85443600
Be	-0.93496600	0.12954000	0.01032500
C	-1.22102900	1.85010600	0.04515000
C	-0.03853300	2.83658100	-0.00696100
H	-1.81570000	2.05623100	0.95071900
H	-1.91539900	2.08260900	-0.77845800
H	-0.34358500	3.89120200	0.02299900
H	0.64885400	2.68662000	0.83572700
H	0.55241400	2.70850000	-0.92309400
C	-2.00395500	-1.24473700	-0.02748900
C	-3.51710500	-0.94972900	-0.02780100
H	-1.77769400	-1.91428600	0.82261600
H	-1.76908700	-1.86546800	-0.91225400
H	-4.14146500	-1.85283600	-0.06119700
H	-3.81253800	-0.38909300	0.86600700
H	-3.80117700	-0.33181800	-0.88680400
C	1.36136700	-1.99813300	0.05996200
H	0.94600600	-2.30969200	1.01240500
H	0.78983300	-2.36349400	-0.78699300
H	2.38600500	-2.36943300	-0.02511100

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -329.255207894
E_0 = -329.038627
H = -329.024766
G = -329.077806

0 1

C	1.294979	-0.989801	-0.013787
C	1.404892	0.266571	-0.166832
C	2.099643	-2.218693	0.227392
H	1.952655	-2.929562	-0.590406
H	3.171872	-2.016163	0.320711
H	1.759714	-2.720670	1.137031
C	2.322619	1.430334	-0.236164
H	3.319635	1.094440	0.065480
H	2.389735	1.831222	-1.250914
H	2.018467	2.241648	0.428039
Be	-0.320290	-0.435654	-0.107839
C	-1.790956	-1.309000	0.208135
C	-3.117831	-0.744918	-0.331352
H	-1.866798	-1.416727	1.302389
H	-1.668683	-2.339686	-0.152909
H	-3.984058	-1.357537	-0.051809
H	-3.318449	0.267144	0.038694
H	-3.117593	-0.685416	-1.426467
C	-0.465025	1.376792	-0.497266
C	-0.926030	2.133656	0.749186
H	-1.423668	3.074130	0.484054
H	-0.086177	2.388457	1.403161
H	-1.630440	1.546015	1.342945
H	0.154441	2.002658	-1.133542
H	-1.323241	1.093018	-1.120975

Transition States (Et-Be-Et)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -714.011354944
E_0 = -713.671436
H = -713.650408
G = -713.722818

0 1

C	-0.38467500	-1.36280500	-0.19318700
C	0.54245800	-0.29927900	-0.15718200
H	-0.00154900	-2.38621500	-0.25112600
H	0.02279300	-0.63588100	-1.26466000
Be	0.20618500	1.48590100	-0.03755800
C	0.31648200	2.03659900	1.63245800
C	-0.49789300	3.27736500	2.04898700
H	1.38960800	2.26509300	1.75991300
H	0.13277100	1.22987300	2.35832200
H	-0.30756700	3.58630300	3.08583800
H	-0.27639700	4.13712900	1.41037600
H	-1.57811100	3.10148100	1.96880300
C	-0.08085800	2.30210600	-1.56804200
C	-0.32187300	3.82449600	-1.56945500
H	-0.93669000	1.81210000	-2.06622600
H	0.76256900	2.08563000	-2.24696100
H	-0.47455200	4.23633800	-2.57630400
H	-1.20324400	4.09302200	-0.97778200
H	0.52391000	4.36376000	-1.12886200
C	1.97464500	-0.69327400	-0.09822600
C	2.41753400	-1.65403600	0.82517300
C	2.92442300	-0.05201700	-0.90968800
C	3.76903500	-1.97298400	0.92485700
H	1.70502200	-2.12935800	1.49107200
C	4.27071600	-0.39316000	-0.82740800
H	2.59821800	0.70868600	-1.60951900
C	4.69790600	-1.35135100	0.09190600
H	4.09722300	-2.70478500	1.65451100
H	4.98969000	0.09921000	-1.47236000
H	5.74965300	-1.60323600	0.16653000
C	-1.84984300	-1.26479700	-0.11270500
C	-2.50168200	-0.11156200	0.35205100
C	-2.61768000	-2.38046100	-0.48704100
C	-3.89000300	-0.07386300	0.41731600
H	-1.92343200	0.74020100	0.68992800
C	-4.00501400	-2.33814000	-0.42228000
H	-2.11940800	-3.28054400	-0.83238600
C	-4.64318500	-1.18144000	0.02679400
H	-4.38489200	0.81863200	0.78167700
H	-4.58791300	-3.20273500	-0.71758100
H	-5.72539700	-1.14668800	0.08106200

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -714.052984178
E_0 = -713.707408
H = -713.687299
G = -713.756754

0 1

C	-0.473465	-0.354345	-0.584104
C	0.531138	-0.282397	0.468525
H	-0.097250	-0.649344	-1.558840
H	0.216501	-0.640463	1.444712
Be	-0.205117	1.358240	-0.324785
C	-0.642028	2.788049	-1.175204
C	0.009313	4.135959	-0.813789
H	-1.736418	2.885153	-1.099027
H	-0.478517	2.589249	-2.245780
H	-0.366318	4.963819	-1.426540
H	-0.169942	4.413930	0.231121
H	1.096974	4.113146	-0.951645
C	0.828830	1.575984	1.293626
C	-0.263191	2.089077	2.239223
H	0.152822	2.824715	2.936822
H	-0.679880	1.275915	2.839868
H	-1.093785	2.573519	1.718592
H	1.621944	1.101194	1.861919
H	1.315151	2.385671	0.736673
C	-1.870905	-0.764833	-0.320404
C	-2.461470	-0.771047	0.955730
C	-2.680358	-1.159811	-1.403628
C	-3.787506	-1.160161	1.139106
H	-1.889364	-0.468224	1.825335
C	-4.002307	-1.545904	-1.220155
H	-2.255552	-1.165254	-2.402294
C	-4.569641	-1.550176	0.055395
H	-4.209444	-1.155464	2.138648
H	-4.593734	-1.848476	-2.077817
H	-5.600968	-1.850424	0.199437
C	1.936734	-0.670175	0.139259
C	2.651850	-1.476779	1.032807
C	2.565841	-0.268634	-1.047240
C	3.952498	-1.885215	0.744247
H	2.181971	-1.796756	1.957274
C	3.868410	-0.667691	-1.331575
H	2.041020	0.361677	-1.757525
C	4.566559	-1.480342	-0.438562
H	4.484570	-2.518872	1.444910
H	4.339053	-0.344020	-2.253112
H	5.579828	-1.792990	-0.663145

Transition States (Et-Be-Et)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -712.785013123
E_0 = -712.466361
H = -712.445343
G = -712.519310

0 1

C	0.50778000	-0.39557300	-0.14243300
C	-0.74629800	-0.48039600	-0.03839200
Be	-2.43113500	-1.18322900	-0.14214400
C	-2.62050400	-2.63554500	0.81580200
H	-3.29217700	-3.30532600	0.25700700
H	-3.21194700	-2.34185300	1.70021200
C	-3.53116000	-0.28210200	-1.14752200
H	-3.09072400	-0.13209700	-2.14864400
H	-3.62476000	0.74273100	-0.74738100
C	-1.39043000	-3.43227100	1.28508200
H	-1.64431500	-4.32043800	1.87929000
H	-0.79328600	-3.78650600	0.43475600
H	-0.72447200	-2.81839200	1.90444800
C	-4.94474100	-0.87616600	-1.31716400
H	-5.60368500	-0.26415900	-1.94832200
H	-4.90673400	-1.87384500	-1.76877000
H	-5.44670900	-0.99416100	-0.35027800
C	1.92779500	-0.54296500	-0.25122800
C	2.75227400	0.48053400	-0.74456400
C	2.49399000	-1.77578900	0.12248700
C	4.12077900	0.27000200	-0.86401000
H	2.31670100	1.43251500	-1.02126300
C	3.86197800	-1.97800700	-0.01808700
H	1.85566700	-2.55971800	0.51119100
C	4.67809500	-0.95801600	-0.50683200
H	4.75398300	1.06532000	-1.23958900
H	4.29234300	-2.93182300	0.26399700
H	5.74554000	-1.11804400	-0.60519000
C	-0.69187800	3.36702400	-0.56264000
C	-0.52202400	3.83291100	0.74334200
C	-0.30482100	2.93458300	1.78962700
C	-0.25739900	1.56922100	1.53591400
C	-0.42969800	1.09582800	0.22358800
C	-0.63898400	2.00485000	-0.82892000
H	-0.86795200	4.06716200	-1.37092300
H	-0.56250100	4.89709000	0.94573500
H	-0.17739700	3.29916100	2.80222900
H	-0.09734500	0.85994500	2.33882900
H	-0.78422500	1.62662000	-1.83305900

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -712.822204073
E_0 = -712.499557
H = -712.479670
G = -712.549742

0 1

C	-0.760685	0.242898	0.076033
C	0.514805	0.316422	0.121198
Be	-0.428559	1.918160	-0.061703
C	1.338576	2.391503	0.306241
C	2.071011	2.858093	-0.947426
H	2.016442	1.914423	1.007582
H	0.890233	3.238442	0.845659
H	2.888836	3.543267	-0.693806
H	2.517023	2.016466	-1.485097
H	1.405572	3.382347	-1.637904
C	-1.471809	3.252471	-0.455040
C	-2.127716	3.888963	0.790815
H	-2.261393	2.947123	-1.153780
H	-0.897082	4.028407	-0.981934
H	-2.751239	4.757424	0.544159
H	-2.768511	3.175997	1.321827
H	-1.379765	4.237458	1.513788
C	1.788268	-0.392444	0.114738
C	2.336215	-0.834297	-1.098800
C	2.451936	-0.698125	1.313030
C	3.520467	-1.567509	-1.110907
H	1.824511	-0.608255	-2.026857
C	3.634067	-1.431329	1.295181
H	2.031067	-0.365090	2.254795
C	4.172789	-1.865935	0.083834
H	3.932886	-1.905036	-2.055047
H	4.134479	-1.666091	2.227862
H	5.094676	-2.436160	0.072513
C	-1.831501	-0.744883	0.006323
C	-3.168654	-0.327577	-0.064761
C	-1.555079	-2.123614	0.013392
C	-4.201432	-1.259310	-0.128035
H	-3.384292	0.733991	-0.071555
C	-2.587865	-3.052766	-0.048139
H	-0.525835	-2.459276	0.067994
C	-3.914142	-2.623342	-0.119534
H	-5.230128	-0.921085	-0.183248
H	-2.360490	-4.113110	-0.041124
H	-4.718250	-3.349184	-0.167882

Transition States (Ph-Be-Ph)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -635.377899688
E_0 = -635.091779
H = -635.073687
G = -635.139061

0 1

C	0.24470900	3.02825300	0.57380900
C	-0.06570000	2.14014200	-0.45358300
H	0.09142300	4.10368000	0.41725400
H	1.14002100	2.38731600	-0.29780900
C	0.73280200	2.63593300	1.93359500
H	1.53787400	3.28934600	2.27812700
H	-0.10517000	2.76179000	2.62945400
H	1.05312600	1.59388100	1.96933800
C	-0.62026900	2.72687600	-1.73100200
H	-1.67383000	2.43750800	-1.78746900
H	-0.55825400	3.82032000	-1.78895600
H	-0.13846900	2.29332900	-2.61039700
Be	-0.02457400	0.32304800	-0.24431900
C	1.53825100	-0.43661300	-0.15940000
C	1.73907700	-1.62727000	0.57240100
C	2.69157000	0.08846700	-0.78095700
C	2.98767800	-2.24092200	0.68559600
H	0.89220000	-2.09026600	1.07236600
C	3.94718100	-0.51622300	-0.69136700
H	2.61773300	0.99719100	-1.38086800
C	4.09885500	-1.68646800	0.05052700
H	3.09537500	-3.15329000	1.26438000
H	4.80304600	-0.07974500	-1.19750900
H	5.07068200	-2.16233600	0.13018700
C	-1.60807600	-0.38059200	-0.10324000
C	-2.74979700	0.32696600	0.32594500
C	-1.82141900	-1.73848700	-0.42451000
C	-4.00952100	-0.26431800	0.43911700
H	-2.66316300	1.38096500	0.58966600
C	-3.07528100	-2.34479300	-0.33013700
H	-0.98292900	-2.34219500	-0.76194000
C	-4.17585000	-1.60795600	0.10627600
H	-4.85946700	0.31879900	0.78111300
H	-3.19509000	-3.39143100	-0.59338700
H	-5.15207600	-2.07504000	0.18529400

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -635.411868394
E_0 = -635.121042
H = -635.103889
G = -635.166668

0 1

C	-0.425151	2.548599	0.034106
C	-1.636275	1.834810	-0.318679
H	0.029901	3.081505	-0.801527
H	-2.426575	1.848876	0.426286
C	-0.362144	3.295907	1.364744
H	0.667832	3.554667	1.622878
H	-0.940709	4.229399	1.347774
H	-0.750908	2.693782	2.192780
C	-2.148476	1.928329	-1.740422
H	-2.509001	2.951516	-1.891825
H	-1.353280	1.756678	-2.470790
H	-2.966397	1.236684	-1.943644
Be	0.095370	0.880683	0.018747
C	-1.453786	-0.145921	-0.029188
C	-1.874479	-0.547953	1.250309
C	-1.650476	-1.040256	-1.093433
C	-2.432199	-1.806226	1.468303
H	-1.763323	0.126628	2.095552
C	-2.219999	-2.294506	-0.884990
H	-1.340776	-0.767750	-2.097304
C	-2.611574	-2.680974	0.397289
H	-2.735923	-2.098756	2.467602
H	-2.354581	-2.972628	-1.720900
H	-3.057285	-3.655968	0.559708
C	1.620670	0.102195	-0.027445
C	2.806483	0.864597	-0.081557
C	1.784436	-1.296995	-0.006313
C	4.071264	0.276090	-0.117108
H	2.742391	1.949765	-0.097901
C	3.041944	-1.900867	-0.037751
H	0.907060	-1.936766	0.035847
C	4.191317	-1.112951	-0.094480
H	4.961041	0.896614	-0.161161
H	3.127974	-2.982951	-0.018437
H	5.171739	-1.577305	-0.120248

Transition States (Ph-Be-Ph)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.140594366
E_0 = -633.875531
H = -633.857387
G = -633.923712

0 1

C	-0.11253700	3.19956600	-0.13623000
C	-0.01884000	1.96593200	0.00876900
C	-0.44559000	4.58687700	-0.44575300
H	0.38719700	5.10673600	-0.92629100
H	-1.29241100	4.57826800	-1.13667500
H	-0.74298100	5.13665800	0.45090500
Be	-0.06576900	0.15506100	-0.03379300
C	1.23714300	2.74509800	1.03870300
H	0.87441800	2.64533600	2.05654000
H	2.00102700	2.01207900	0.78855500
H	1.66053700	3.73765500	0.87257300
C	1.50389100	-0.59016300	-0.04681300
C	2.58625900	-0.09223200	-0.80379100
C	1.77645600	-1.75211900	0.70611300
C	3.84322400	-0.70106300	-0.82004200
H	2.44582000	0.79370600	-1.42341900
C	3.03036200	-2.36632300	0.71491200
H	0.98429700	-2.19560600	1.30459300
C	4.07048600	-1.84222500	-0.05198400
H	4.64240400	-0.29003300	-1.42986800
H	3.19561800	-3.25724900	1.31328200
H	5.04481000	-2.31973200	-0.05471000
C	-1.65219200	-0.52719500	-0.04410300
C	-1.84823100	-1.88655500	-0.37201500
C	-2.82249700	0.19943900	0.26127900
C	-3.11163300	-2.47848000	-0.39597000
H	-0.98651800	-2.50092100	-0.61979700
C	-4.09391400	-0.37670200	0.24896100
H	-2.74440700	1.25303000	0.52396700
C	-4.24154100	-1.72287500	-0.08286800
H	-3.21765200	-3.52712900	-0.65712900
H	-4.96771400	0.21940000	0.49536600
H	-5.22644500	-2.17832800	-0.09772500

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -634.184669510
E_0 = -633.917349
H = -633.900130
G = -633.963347

0 1

C	0.643894	3.754449	-0.000320
C	-0.121320	2.478399	-0.000155
C	-1.292854	2.000742	0.000095
C	-2.757283	2.233783	0.000444
H	-3.234765	1.803721	0.882233
H	-2.919892	3.317255	0.000602
H	-3.235162	1.803910	-0.881221
C	-1.376568	-0.143700	-0.000033
C	-1.844275	-0.695627	-1.203595
C	-2.720239	-1.780411	-1.206378
C	-3.162322	-2.323853	0.000088
C	-2.719569	-1.780827	1.206497
C	-1.843589	-0.696061	1.203599
H	-1.510321	-0.286457	2.153228
H	-3.056267	-2.202670	2.147695
H	-3.846716	-3.164995	0.000133
H	-3.057474	-2.201931	-2.147531
H	-1.511613	-0.285660	-2.153280
Be	0.165000	0.771769	-0.000140
C	1.673507	-0.061031	-0.000083
C	1.742250	-1.468050	-0.000451
C	2.957537	-2.154257	-0.000410
C	4.158053	-1.445016	-0.000002
C	4.130731	-0.050975	0.000369
C	2.907346	0.620751	0.000322
H	2.920382	1.707461	0.000593
H	5.060656	0.509456	0.000582
H	5.105817	-1.973407	0.000008
H	2.969847	-3.239900	-0.000713
H	0.822689	-2.046951	-0.000793
H	-0.008228	4.633382	-0.001442
H	1.293815	3.805433	0.876894
H	1.295440	3.804373	-0.876364

Transition States (Ph-Be-Ph)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1018.94258264
E_0 = -1018.550361
H = -1018.526207
G = -1018.607737

0 1

C	0.24437900	-1.78211100	-1.12997000
C	-0.61969200	-0.93128400	-0.41313800
H	-0.16574200	-2.71661200	-1.52362100
H	0.13060200	-1.71407300	0.23526600
Be	-0.18080700	0.62947100	0.41127200
C	0.53617900	0.42832700	1.98937100
C	1.52912200	1.30962600	2.46825500
C	0.18819400	-0.62252100	2.86565400
C	2.13604700	1.15456400	3.71546300
H	1.83870600	2.14774600	1.84859700
C	0.77448700	-0.78683000	4.12268600
H	-0.58800800	-1.33129200	2.57818600
C	1.75825900	0.10280200	4.55030400
H	2.89895000	1.85565400	4.04066300
H	0.46421900	-1.60344500	4.76785100
H	2.22204000	-0.01877200	5.52370800
C	-0.47771800	2.11379100	-0.45378600
C	-0.64824200	2.19645000	-1.85195300
C	-0.57194900	3.33806900	0.24266500
C	-0.88576100	3.40187600	-2.51514700
H	-0.59341600	1.29066300	-2.45421500
C	-0.81930200	4.55178000	-0.40150300
H	-0.45274000	3.34375500	1.32284200
C	-0.97401900	4.58774300	-1.78696900
H	-1.00426300	3.41805800	-3.59450300
H	-0.88959600	5.46944900	0.17478000
H	-1.16254200	5.52873400	-2.29346400
C	-2.03154700	-1.40038000	-0.27575300
C	-3.06092700	-0.46804600	-0.47423900
C	-2.37768400	-2.72367700	0.04666300
C	-4.39518400	-0.86009000	-0.39234700
H	-2.80864000	0.56005800	-0.70442700
C	-3.71147400	-3.10522500	0.15191700
H	-1.60358000	-3.45747900	0.24937200
C	-4.72581200	-2.17603200	-0.07701200
H	-5.17683900	-0.12873900	-0.56357900
H	-3.95868800	-4.12658800	0.41890200
H	-5.76496800	-2.47402700	0.00288300
C	1.66299000	-1.57351700	-1.44966500
C	2.39913700	-2.67384000	-1.92171100
C	2.29671400	-0.32581300	-1.33312100
C	3.74293800	-2.53902500	-2.24779700
H	1.91145300	-3.63743000	-2.02751900
C	3.64036700	-0.19504500	-1.66185400
H	1.73851800	0.54677500	-1.01593900
C	4.36575800	-1.29817000	-2.11382000
H	4.30231300	-3.39485000	-2.60677000
H	4.12048500	0.77218700	-1.57312000
H	5.41339200	-1.18818700	-2.37014600

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1018.980937530
E_0 = -1018.584413
H = -1018.561020
G = -1018.639385

0 1

C	-1.036057	-0.722079	-0.784408
C	0.076916	-1.367972	-0.106513
H	-0.900658	-0.584667	-1.853486
H	-0.180299	-2.090270	0.658892
Be	-0.162538	0.611045	0.000603
C	0.802392	-0.175205	1.353388
C	-0.013879	-0.088777	2.496776
C	2.192246	-0.090066	1.519071
C	0.541103	0.133558	3.757110
H	-1.093172	-0.170085	2.408295
C	2.748187	0.114528	2.778699
H	2.845621	-0.179707	0.658264
C	1.923783	0.229278	3.900072
H	-0.105070	0.220530	4.623773
H	3.824928	0.186870	2.888162
H	2.359120	0.386653	4.880567
C	0.060711	2.253871	-0.420859
C	-0.661606	2.838746	-1.481754
C	0.959648	3.101167	0.257550
C	-0.498744	4.175204	-1.848226
H	-1.376460	2.237271	-2.037602
C	1.133122	4.439700	-0.095652
H	1.542288	2.707646	1.086137
C	0.402849	4.980574	-1.153383
H	-1.073869	4.589638	-2.670384
H	1.835035	5.061457	0.451433
H	0.533514	6.021011	-1.432288
C	-2.447816	-0.957327	-0.390460
C	-3.470484	-0.447709	-1.213603
C	-2.844120	-1.668742	0.755371
C	-4.812944	-0.635515	-0.907949
H	-3.199184	0.103712	-2.108088
C	-4.191009	-1.854954	1.063553
H	-2.102887	-2.099456	1.419218
C	-5.186488	-1.339250	0.237868
H	-5.572573	-0.229309	-1.567237
H	-4.460238	-2.413392	1.953899
H	-6.233003	-1.484519	0.479183
C	1.276970	-1.782564	-0.889734
C	1.890461	-3.005764	-0.591169
C	1.798604	-1.007237	-1.935080
C	2.981082	-3.456145	-1.330529
H	1.505116	-3.611644	0.222322
C	2.897929	-1.451154	-2.664818
H	1.356527	-0.046978	-2.178151
C	3.490013	-2.678728	-2.369223
H	3.434326	-4.411904	-1.092821
H	3.291442	-0.836762	-3.466631
H	4.342451	-3.024912	-2.942458

Transition States (Ph-Be-Ph)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1017.71622135
E_0 = -1017.345039
H = -1017.321038
G = -1017.403057

0 1

C	-1.55052000	-0.01711700	-0.05476400
C	-0.30145700	-0.06120500	0.11026000
Be	1.39745200	0.59354500	0.04242200
C	-2.94678700	0.26346400	-0.20275700
C	-3.46294500	1.41258300	0.42300600
C	-3.79136700	-0.54974900	-0.97568600
C	-4.80249600	1.74560800	0.25731100
H	-2.80762200	2.03498600	1.01984700
C	-5.13116800	-0.21343600	-1.12089600
H	-3.39419400	-1.43973600	-1.44790700
C	-5.63812700	0.93418700	-0.50932200
H	-5.19503500	2.63627700	0.73364200
H	-5.78153700	-0.84515800	-1.71442600
H	-6.68368100	1.19365800	-0.62884300
C	-1.18953000	-3.49765500	1.73877100
C	-0.99168800	-4.36357400	0.66095000
C	-0.69352100	-3.85857800	-0.60605500
C	-0.59853200	-2.48667200	-0.80311700
C	-0.78590900	-1.61306700	0.28121800
C	-1.08867100	-2.12469100	1.55424400
H	-1.41733600	-3.89461800	2.72105600
H	-1.06564100	-5.43471100	0.81022500
H	-0.52926800	-4.53481800	-1.43660800
H	-0.35019800	-2.08009000	-1.77566900
H	-1.23250800	-1.44079500	2.38200100
C	2.71096900	-0.51443600	-0.16560500
C	2.78946000	-1.78357900	0.44663800
C	3.80886800	-0.16956400	-0.98409800
C	3.87547400	-2.64317400	0.26940100
H	1.98319600	-2.11807600	1.09632000
C	4.89509500	-1.02235600	-1.18779900
H	3.81795600	0.79920000	-1.47783800
C	4.93323200	-2.26557200	-0.55687400
H	3.89823500	-3.60567200	0.77237800
H	5.71497100	-0.71644200	-1.83091200
H	5.77842300	-2.93017500	-0.70438000
C	1.41975800	2.32853900	0.14407900
C	2.57549300	2.99280600	0.60810800
C	0.34498700	3.16382700	-0.22185900
C	2.65345400	4.38326000	0.70742800
H	3.44280100	2.40605000	0.89962400
C	0.40869300	4.55624700	-0.14347700
H	-0.57637600	2.72063600	-0.59661800
C	1.56762000	5.17186100	0.32849400
H	3.56137200	4.85270900	1.07432600
H	-0.44013600	5.16143100	-0.44874600
H	1.62446300	6.25341800	0.39724600

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1017.748381980
E_0 = -1017.375238
H = -1017.351908
G = -1017.431555

0 1

C	-0.302575	1.084323	0.053091
C	0.828279	0.516678	-0.073059
C	0.706290	-1.670035	0.082429
C	1.258202	-2.074337	1.307343
C	2.006056	-3.247224	1.408149
C	2.240037	-4.024013	0.274211
C	1.711226	-3.630246	-0.956054
C	0.955577	-2.463409	-1.049750
H	0.533050	-2.186662	-2.011236
H	1.881148	-4.237471	-1.839074
H	2.829950	-4.930965	0.347797
H	2.411474	-3.550217	2.367755
H	1.103534	-1.472264	2.198246
Be	-0.728512	-0.602097	0.041943
C	-2.304724	-1.297515	-0.052795
C	-2.551558	-2.601679	0.418934
C	-3.813855	-3.192538	0.345724
C	-4.877589	-2.495182	-0.225699
C	-4.667977	-1.206437	-0.714624
C	-3.404293	-0.621171	-0.618142
H	-3.276304	0.387077	-1.002289
H	-5.488572	-0.657570	-1.166497
H	-5.859362	-2.952576	-0.291540
H	-3.966888	-4.197941	0.725866
H	-1.737256	-3.176872	0.851670
C	-0.938508	2.394837	0.064740
C	-2.167803	2.582200	0.713919
C	-0.329959	3.494558	-0.565710
C	-2.763572	3.840050	0.749171
H	-2.647536	1.735177	1.188752
C	-0.938879	4.744561	-0.545183
H	0.617661	3.359465	-1.074065
C	-2.154638	4.922739	0.116676
H	-3.709421	3.971784	1.262451
H	-0.462764	5.582824	-1.041700
H	-2.624858	5.899477	0.135877
C	2.277867	0.664765	-0.104247
C	3.077004	0.166915	-1.142087
C	2.874243	1.428699	0.912356
C	4.441319	0.433206	-1.164141
H	2.627728	-0.430583	-1.924262
C	4.242101	1.685055	0.888494
H	2.259124	1.818082	1.714817
C	5.029074	1.188718	-0.148870
H	5.049003	0.047477	-1.974738
H	4.691618	2.271720	1.681655
H	6.094642	1.387319	-0.166513

Transition States (Ph-Be-Ph)

(1,1)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -786.608637209
E_0 = -786.320487
H = -786.301118
G = -786.371700

0 1

C	-1.85616500	0.01130700	0.00508700
C	-0.60914000	-0.08934100	-0.04286100
Be	1.18388100	-0.02510300	-0.04632100
C	-3.29412100	-0.04436800	0.01858200
C	-3.94855100	-0.91534000	-0.86622500
C	-4.03556100	0.74155800	0.91347000
C	-5.33588400	-1.00168600	-0.84275900
H	-3.36864100	-1.51407900	-1.55761200
C	-5.42253500	0.65582700	0.91689800
H	-3.52537700	1.40639600	1.60027700
C	-6.07269100	-0.21598800	0.04319600
H	-5.84178900	-1.67828400	-1.52108400
H	-5.99591000	1.26441800	1.60581100
H	-7.15435400	-0.28301000	0.05316900
C	1.78660800	1.60263600	-0.06362200
C	1.13663000	2.67285300	-0.71237000
C	2.98746000	1.93441700	0.59948100
C	1.63760400	3.97618300	-0.71239400
H	0.21403900	2.49221700	-1.26612100
C	3.49755400	3.23320700	0.62225400
H	3.54121700	1.15533100	1.11685700
C	2.82335300	4.26080000	-0.03719200
H	1.10844900	4.76620200	-1.23679900
H	4.42251100	3.44506100	1.14992800
H	3.21885700	5.27108700	-0.02709200
C	1.96874400	-1.56114300	0.00094100
C	3.32973700	-1.68639700	-0.35168500
C	1.32439200	-2.75790400	0.38006200
C	4.00038900	-2.90991800	-0.32989600
H	3.88271600	-0.80193600	-0.65704100
C	1.98105500	-3.98885000	0.41587600
H	0.27421200	-2.73562600	0.66650200
C	3.32616100	-4.06775900	0.05743900
H	5.04747500	-2.96236000	-0.61244200
H	1.44765000	-4.88461800	0.71968900
H	3.84341000	-5.02145500	0.07914800
H	-1.20023600	1.08048900	-0.01358700

(1,2)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -786.63320658
E_0 = -786.341787
H = -786.323092
G = -786.391383

0 1

C	0.967877	-1.233560	-0.021007
C	-0.023277	-1.996463	-0.161088
C	-1.989365	-1.125534	-0.040555
C	-2.596021	-1.421751	1.190237
C	-3.945666	-1.769566	1.261605
C	-4.706035	-1.855360	0.096357
C	-4.112895	-1.585230	-1.138171
C	-2.766918	-1.231419	-1.205149
H	-2.324959	-1.021871	-2.174800
H	-4.701064	-1.648424	-2.047663
H	-5.752659	-2.134114	0.148043
H	-4.400160	-1.979227	2.224183
H	-2.016227	-1.375013	2.107987
Be	-0.467776	-0.188885	-0.049394
C	-0.480439	1.531542	-0.081305
C	-1.602928	2.245897	0.382030
C	-1.658008	3.640148	0.358510
C	-0.586327	4.371104	-0.152434
C	0.536083	3.697326	-0.632218
C	0.585017	2.303194	-0.586509
H	1.476949	1.809892	-0.962500
H	1.372706	4.257756	-1.037930
H	-0.626551	5.455055	-0.179305
H	-2.537840	4.155983	0.730420
H	-2.460945	1.702227	0.768289
C	2.410560	-1.084843	0.047670
C	3.250495	-1.992042	-0.621544
C	2.988072	-0.044332	0.789900
C	4.632342	-1.857033	-0.547851
H	2.811077	-2.795660	-1.200978
C	4.372236	0.073085	0.877822
H	2.345033	0.666509	1.293797
C	5.197265	-0.827679	0.206320
H	5.269965	-2.558811	-1.073672
H	4.806223	0.875871	1.462906
H	6.275067	-0.727776	0.267116
H	-0.497924	-2.951758	-0.264041

Transition States ($B(C_6F_5)_3$)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2364.90284705
E_0 = -2364.665381
H = -2364.629886
G = -2364.732933

0 1

C	-0.41143800	0.41767300	3.28057500
C	-0.07175800	0.04932800	2.14724700
C	-0.91844000	1.01153100	4.50852400
H	-1.60336400	1.81070400	4.21208500
H	-1.46900500	0.28579500	5.11212500
H	-0.11389100	1.44846900	5.10512400
C	0.84872800	-0.93841300	3.29827000
H	0.43317600	-1.25599700	4.25497500
H	0.81907300	-1.81585200	2.65741500
H	1.83812500	-0.50837000	3.39968400
C	1.41864000	-0.79236500	0.09961200
C	2.63019300	-0.33829200	0.62256900
C	1.54532300	-1.86551700	-0.78272200
C	3.86904500	-0.88401300	0.32354900
C	2.76756000	-2.44513400	-1.11544800
C	3.93889700	-1.95407800	-0.55905400
C	-0.03933300	1.53962800	0.01503900
C	0.77913600	2.09400000	-0.97079700
C	-0.96395200	2.43487900	0.55131900
C	0.70761000	3.42367700	-1.37306800
C	-1.07173100	3.76869500	0.18378800
C	-0.22113400	4.27270600	-0.78926700
B	0.00852500	-0.04381700	0.50512200
C	-1.34285300	-0.86013300	0.01111000
C	-2.06996000	-0.52719200	-1.13355500
C	-1.84370700	-1.96453200	0.69637600
C	-3.21003100	-1.20828300	-1.54739800
C	-2.97574900	-2.67524400	0.32453200
C	-3.67278200	-2.28930100	-0.81115300
F	0.46815800	-2.40105000	-1.38923700
F	2.82011300	-3.47365200	-1.96940400
F	5.11724800	-2.50203100	-0.86454200
F	4.98846600	-0.39247200	0.87114500
F	2.63208700	0.72021800	1.47423900
F	-1.67359000	0.48164300	-1.93454400
F	-3.86058100	-0.83387600	-2.65515100
F	-4.76679100	-2.95292700	-1.19305800
F	-3.39379300	-3.72571400	1.04416300
F	-1.19332600	-2.43192100	1.79739300
F	-1.85082800	2.01075300	1.49267200
F	-1.98408300	4.56641900	0.75709500
F	-0.30065400	5.55260100	-1.16191900
F	1.52435300	3.88981700	-2.32511800
F	1.68429500	1.34070200	-1.62676700

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2364.90422231
E_0 = -2364.666423
H = -2364.631316
G = -2364.732634

0 1

B	-0.21747100	-0.09558000	0.74314000
C	-0.40341900	0.17935800	2.36244800
C	-0.06410100	1.40934400	2.30289300
C	0.00872100	2.79703100	2.75191200
H	-0.32472900	2.77592600	3.79881700
H	-0.67400200	3.44320200	2.19613700
H	1.01985600	3.20702200	2.72394000
C	0.56717000	1.41639600	0.30517600
C	1.95561800	1.56268200	0.52437600
C	0.02771000	2.36348500	-0.58727500
C	2.73483000	2.54465800	-0.06517300
C	0.77861800	3.35693900	-1.19844000
C	2.14110900	3.45077100	-0.93668300
C	-1.02149600	-0.60919400	3.48163400
H	-0.25113800	-1.16099300	4.02047900
H	-1.54662600	0.04090800	4.18432800
H	-1.72611300	-1.33849300	3.07888000
C	0.86735800	-1.24121500	0.30774300
C	1.35635100	-1.26982600	-1.00112700
C	1.39061800	-2.22846100	1.13578800
C	2.28611200	-2.18756600	-1.46325700
C	2.32251300	-3.17314000	0.71722800
C	2.77678000	-3.15317800	-0.59223500
C	-1.74585900	-0.31380400	0.14772900
C	-2.12035000	-1.41202000	-0.63749000
C	-2.82609500	0.51487500	0.48489100
C	-3.42168900	-1.65576000	-1.07050500
C	-4.13551200	0.30855300	0.07457600
C	-4.44165300	-0.78954000	-0.71576000
F	-1.26568600	2.33642800	-0.92152600
F	0.21140800	4.21691200	-2.04739200
F	2.86815100	4.40219200	-1.50949600
F	4.04107100	2.63708100	0.19900200
F	2.59517200	0.73954000	1.36767400
F	0.89382800	-0.37597100	-1.90453600
F	2.70406400	-2.16210500	-2.73462800
F	3.67117100	-4.05032800	-1.01308700
F	2.78585600	-4.09603400	1.56989100
F	1.00646100	-2.31923700	2.42778200
F	-1.22374300	-2.33779100	-1.03034000
F	-2.64313100	1.61680500	1.24972500
F	-5.10361000	1.16096000	0.43532400
F	-5.69432400	-1.00770200	-1.11992000
F	-3.69223500	-2.72875100	-1.82280500

Transition States ($B(C_6F_5)_3$)

(1,1)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2517.36889458
E_0 = -2517.108529
H = -2517.071399
G = -2517.181451

0 1

C	2.41230500	0.48725600	-1.10020400
C	1.29612300	0.26776200	-0.59940100
C	-0.93407500	1.48158100	0.01783200
C	-0.27605500	2.60129800	0.53081800
C	-2.23029500	1.73100400	-0.43276200
C	-0.82943300	3.87214400	0.58587400
C	-2.82514100	2.98880700	-0.39513500
C	-2.12031000	4.06925300	0.11412100
C	0.13125200	-0.60054200	1.49374900
C	-0.52132900	-0.19871900	2.66046900
C	1.07316400	-1.61266000	1.67964800
C	-0.25432200	-0.74413100	3.91179000
C	1.37227600	-2.18326600	2.90875500
C	0.70216500	-1.74136900	4.04054100
B	-0.18812300	0.01186000	-0.01028200
C	-0.92557200	-1.08414600	-0.99749500
C	-1.70121200	-2.15156700	-0.54462200
C	-0.83940500	-0.99267400	-2.38413700
C	-2.32049200	-3.06250200	-1.39445300
C	-1.43500200	-1.87431100	-3.27311900
C	-2.18478600	-2.92811600	-2.76908800
F	-3.00029700	0.73775900	-0.92085500
F	-4.07351900	3.16357000	-0.84446600
F	-2.67620200	5.28252100	0.15397800
F	-0.13743500	4.90169600	1.09077600
F	0.97292300	2.47028300	1.03736900
F	-1.91721100	-2.33771400	0.77123000
F	-3.05207800	-4.06517400	-0.89722200
F	-2.77259300	-3.79510400	-3.59600500
F	-1.29857800	-1.71719300	-4.59533800
F	-0.14513900	0.04235000	-2.95097000
F	1.74979800	-2.10918300	0.61271500
F	2.29512200	-3.14921500	3.00949000
F	0.97101400	-2.27176700	5.23534700
F	-0.91719700	-0.31902200	4.99290200
F	-1.48900100	0.73623400	2.62661000
C	3.79772800	0.63110200	-1.46659600
C	4.72066500	-0.30782000	-0.98070900
C	4.22294800	1.69365100	-2.27646800
C	6.06639100	-0.16876400	-1.30004800
H	4.37816300	-1.12936400	-0.36381500
C	5.56980900	1.81279400	-2.59725700
H	3.50579000	2.41919700	-2.64146000
C	6.49058400	0.88586600	-2.10829700
H	6.78297800	-0.88814200	-0.92226900
H	5.90177700	2.63195300	-3.22361300
H	7.54043900	0.98581900	-2.35797700
H	1.49711700	0.55927500	-1.91235700

(1,2)-phenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2517.36926165
E_0 = -2517.105918
H = -2517.069455
G = -2517.175440

0 1

B	0.39904100	0.02961300	-0.58115800
C	-0.34046300	0.12626000	-2.01613700
C	-1.58024600	0.09111700	-1.64637700
C	-1.11875100	-0.17711100	0.28914100
C	-1.62786400	-1.46659100	0.56851200
C	-1.70452500	0.85824400	1.05347400
C	-2.60137600	-1.71930000	1.51560100
C	-2.67649900	0.64470200	2.01167800
C	-3.12279400	-0.65526300	2.24731100
C	1.42636100	-1.23758000	-0.43958400
C	1.58268100	-2.06896600	0.67041600
C	2.32209100	-1.49604700	-1.48056700
C	2.52898200	-3.08483000	0.74589800
C	3.28252000	-2.49843900	-1.44799000
C	3.38656800	-3.30415500	-0.32232300
C	1.17881400	1.40481200	-0.15570300
C	1.61176700	1.62244100	1.15296000
C	1.53345900	2.41014000	-1.05520200
C	2.33759200	2.73395900	1.55660400
C	2.26147100	3.54002000	-0.69632900
C	2.66848000	3.70429300	0.61965800
F	-1.35886400	2.13037500	0.82969500
F	-3.20737900	1.65637000	2.70183200
F	-4.06666400	-0.87424500	3.15062200
F	-3.05586800	-2.95528000	1.73388400
F	-1.19811400	-2.51511100	-0.14037300
F	0.78625500	-1.93210600	1.75243700
F	2.61778600	-3.85373800	1.83845900
F	4.30339400	-4.27370200	-0.26705300
F	4.10994000	-2.68907900	-2.48343800
F	2.29680100	-0.73310300	-2.59605200
F	1.30066200	0.72424100	2.11156500
F	1.17238400	2.33573400	-2.35484700
F	2.57229300	4.46964200	-1.60921800
F	3.36811500	4.78262100	0.98198500
F	2.71349600	2.88335400	2.83298900
C	-2.99486500	0.16707600	-1.88242700
C	-3.74271700	-0.99912800	-2.13336400
C	-3.63214300	1.42231300	-1.91138000
C	-5.09761000	-0.90462000	-2.42391500
H	-3.24961500	-1.96363300	-2.11390800
C	-4.98821000	1.50531400	-2.20150700
H	-3.05313600	2.31730200	-1.71820600
C	-5.72040500	0.34464800	-2.45573500
H	-5.66879700	-1.80215100	-2.62953800
H	-5.47439500	2.47311800	-2.23319900
H	-6.77836900	0.41345700	-2.68172600
H	0.00706700	0.23025400	-3.03627900

Transition States ($Be(C_6F_5)_2$)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1626.80080089
E_0 = -1626.616626
H = -1626.589609
G = -1626.676172

0 1

C	0.635940	3.771669	-0.145736
C	0.236818	2.599489	-0.032539
C	1.384065	5.007887	-0.344650
H	1.352659	5.645707	0.542154
H	2.422532	4.727232	-0.537927
H	1.009153	5.567587	-1.205078
Be	0.058085	0.835605	-0.007370
C	-1.174709	3.730310	0.123820
H	-1.739676	3.578403	-0.789479
H	-1.602977	3.228272	0.986032
H	-1.113523	4.793464	0.364293
C	-1.558112	0.174737	-0.095078
C	-2.513697	0.397999	0.881657
C	-1.962848	-0.662537	-1.125381
C	-3.785628	-0.158842	0.874296
C	-3.221389	-1.247476	-1.194185
C	-4.138527	-0.993365	-0.179848
C	1.564722	-0.044209	0.090868
C	1.614338	-1.359987	0.545239
C	2.796713	0.482585	-0.278346
C	2.784181	-2.105783	0.631295
C	3.995856	-0.214307	-0.218769
C	3.985390	-1.524981	0.242418
F	-2.207224	1.215958	1.935858
F	-4.669686	0.093176	1.851855
F	-5.357046	-1.543617	-0.221715
F	-3.567882	-2.045904	-2.213625
F	-1.102613	-0.934353	-2.137420
F	0.481434	-1.978980	0.945725
F	2.775593	-3.368055	1.081487
F	5.124300	-2.220727	0.314401
F	5.154421	0.350886	-0.593719
F	2.877682	1.764705	-0.738499

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1626.82572934
E_0 = -1626.639686
H = -1626.613528
G = -1626.697244

0 1

C	0.741713	4.199240	0.713908
C	-0.051962	2.960650	0.464624
C	-1.265660	2.638515	0.251046
C	-2.672100	3.077906	0.086273
H	-3.326595	2.655787	0.851051
H	-2.675710	4.168665	0.187987
H	-3.069249	2.819910	-0.897101
C	-1.510835	0.619134	0.028038
C	-1.890885	0.188948	-1.242123
C	-2.847493	-0.792989	-1.447997
C	-3.467480	-1.370904	-0.342319
C	-3.124945	-0.965486	0.945230
C	-2.162429	0.019624	1.104324
Be	0.163238	1.281630	0.250599
C	1.574196	0.278896	0.159844
C	1.586379	-1.081039	0.450590
C	2.721375	-1.878301	0.370562
C	3.922193	-1.301335	-0.025771
C	3.966961	0.054024	-0.330722
C	2.802109	0.803868	-0.229155
H	0.125938	5.102563	0.708091
H	1.247193	4.124511	1.679874
H	1.525569	4.292461	-0.039866
F	2.902951	2.119191	-0.543180
F	5.124256	0.609939	-0.715585
F	5.027845	-2.045692	-0.113627
F	2.678362	-3.184377	0.667031
F	0.445514	-1.698508	0.844670
F	-1.304530	0.734028	-2.325117
F	-3.179800	-1.194873	-2.678444
F	-4.391511	-2.312257	-0.517800
F	-3.722078	-1.531365	1.997845
F	-1.848445	0.393367	2.358589

Transition States ($Be(C_6F_5)_2$)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2010.37958296
E_0 = -2010.089185
H = -2010.056301
G = -2010.158726

0 1

C	-2.522870	0.061172	-0.312602
C	-1.291116	-0.040059	-0.077088
Be	0.476351	0.131756	-0.139180
C	-3.838264	0.258059	-0.849277
C	-4.927113	0.613247	-0.038203
C	-4.012900	0.126509	-2.238046
C	-6.171381	0.839172	-0.612889
H	-4.792476	0.705741	1.032392
C	-5.260072	0.369309	-2.802464
H	-3.171821	-0.158142	-2.858243
C	-6.339374	0.722096	-1.993398
H	-7.011291	1.110801	0.015522
H	-5.390002	0.275137	-3.874075
H	-7.311649	0.902828	-2.436878
C	-2.544264	-1.094432	3.450850
C	-2.693635	-2.473950	3.296186
C	-2.528776	-3.073988	2.044477
C	-2.213997	-2.296650	0.938999
C	-2.064315	-0.906355	1.092105
C	-2.234465	-0.303485	2.351067
H	-2.664407	-0.639325	4.426726
H	-2.936025	-3.087222	4.156696
H	-2.642288	-4.146050	1.936280
H	-2.071456	-2.741711	-0.038048
H	-2.093435	0.765621	2.450112
C	1.078954	1.771874	-0.087640
C	0.681836	2.680855	0.880369
C	1.995737	2.262133	-1.007528
C	1.147809	3.985953	0.962019
C	2.494687	3.559028	-0.982816
C	2.065480	4.426334	0.015453
C	1.420689	-1.338936	-0.234018
C	1.059309	-2.424727	-1.018668
C	2.613457	-1.498761	0.461826
C	1.806210	-3.590013	-1.131499
C	3.401902	-2.641600	0.393281
C	2.992084	-3.695522	-0.414919
F	0.732564	4.822336	1.927416
F	-0.214699	2.293806	1.835538
F	2.531024	5.680242	0.063557
F	3.375113	3.988797	-1.899162
F	2.437889	1.456657	-2.004393
F	-0.097413	-2.379053	-1.741636
F	1.404944	-4.608918	-1.909904
F	3.731393	-4.807686	-0.498908
F	4.542343	-2.748270	1.091189
F	3.055263	-0.508831	1.273276

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -2010.39169960
E_0 = -2010.100067
H = -2010.067558
G = -2010.168625

0 1

C	-0.393515	1.838416	0.272162
C	-1.415338	1.088628	0.053762
Be	0.437533	0.355644	0.155506
C	2.100366	-0.119494	0.033210
C	2.948823	0.419476	-0.924526
C	2.673795	-1.071102	0.865118
C	4.282015	0.052924	-1.063048
F	2.473834	1.351144	-1.786845
C	4.000834	-1.472124	0.776155
F	1.919100	-1.651686	1.831880
C	4.809377	-0.902052	-0.200964
F	5.062619	0.598877	-2.006334
F	4.510969	-2.391746	1.607329
F	6.089811	-1.270609	-0.310964
C	-0.882338	-0.894454	0.056084
C	-1.051263	-1.585810	-1.143634
C	-1.276972	-1.560715	1.215542
C	-1.576877	-2.865416	-1.205523
F	-0.692850	-0.994406	-2.298512
C	-1.806135	-2.842437	1.199494
F	-1.157720	-0.949477	2.407742
C	-1.956833	-3.494636	-0.021135
F	-1.719428	-3.506204	-2.369840
F	-2.171462	-3.457760	2.328028
F	-2.467281	-4.723218	-0.058463
C	-2.844927	0.977441	-0.202308
C	-3.329190	1.089480	-1.515126
C	-3.748895	0.836898	0.862523
C	-4.699624	1.066855	-1.754120
H	-2.629912	1.196439	-2.335556
C	-5.116970	0.816232	0.613285
H	-3.374123	0.750607	1.875470
C	-5.594064	0.928744	-0.693046
H	-5.068743	1.157102	-2.769125
H	-5.811494	0.713215	1.438967
H	-6.661070	0.909543	-0.883036
C	-0.153484	3.272264	0.428759
C	1.144882	3.734577	0.686194
C	-1.199823	4.206685	0.337078
C	1.393451	5.094289	0.850081
H	1.955544	3.019833	0.756373
C	-0.948859	5.563951	0.500043
H	-2.208655	3.864473	0.138191
C	0.348230	6.011203	0.757425
H	2.402287	5.437454	1.048480
H	-1.763890	6.275176	0.426900
H	0.541587	7.070427	0.884201

Reactants

Et-Mg-Et

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -358.570993592
E_0 = -358.444718
H = -358.434955
G = -358.480721

0 1

C	0.000000	2.121256	0.303729
C	-1.136569	2.819669	-0.472654
H	0.969320	2.461134	-0.086573
H	-0.014451	2.457068	1.349925
H	-1.070520	3.914589	-0.422968
H	-1.131103	2.553905	-1.535665
H	-2.125105	2.547982	-0.085810
C	0.000000	-2.121256	0.303729
C	1.136569	-2.819669	-0.472654
H	-0.969320	-2.461134	-0.086573
H	0.014451	-2.457068	1.349925
H	1.070520	-3.914589	-0.422968
H	1.131103	-2.553905	-1.535665
H	2.125105	-2.547982	-0.085810
Mg	0.000000	0.000000	0.299107

Ph-Mg-Ph

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -663.495325150
E_0 = -663.316833
H = -663.304151
G = -663.357733

0 1

C	-2.095200	0.000015	0.000016
C	-2.841858	0.845793	0.845754
C	-2.841813	-0.845786	-0.845739
C	-4.237989	0.851065	0.851029
H	-2.334414	1.526583	1.526510
C	-4.237944	-0.851100	-0.851049
H	-2.334333	-1.526564	-1.526482
C	-4.940728	-0.000027	-0.000018
H	-4.775941	1.517746	1.517679
H	-4.775860	-1.517797	-1.517711
H	-6.025413	-0.000043	-0.000032
C	2.095200	0.000043	-0.000023
C	2.841877	0.845770	-0.845795
C	2.841795	-0.845732	0.845775
C	4.238008	0.851016	-0.851065
H	2.334446	1.526539	-1.526582
C	4.237926	-0.851070	0.851091
H	2.334301	-1.526469	1.526548
C	4.940728	-0.000050	0.000024
H	4.775974	1.517658	-1.517742
H	4.775828	-1.517747	1.517785
H	6.025413	-0.000085	0.000041
Mg	0.000000	0.000047	-0.000001

Products (Et-Mg-Et)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -515.860152415
E_0 = -515.621591
H = -515.606429
G = -515.664358

0 1

C	1.195448	0.036344	0.025198
C	1.547286	1.325121	-0.748019
C	1.898016	0.053404	1.398230
H	1.597479	0.903482	2.019271
H	1.702107	-0.848598	1.986965
H	2.994392	0.120875	1.277746
C	0.987773	2.634205	-0.176085
H	1.284231	3.492332	-0.786391
H	-0.111330	2.630540	-0.148037
H	1.339999	2.822321	0.841522
C	-3.034168	-0.244211	0.631942
C	-3.943756	0.059637	-0.577296
H	-3.299223	0.423461	1.463482
H	-3.248975	-1.255707	1.003747
H	-5.010834	-0.038410	-0.337628
H	-3.800117	1.078846	-0.953177
H	-3.748804	-0.615946	-1.417752
H	1.205947	1.227752	-1.786958
H	2.646679	1.422292	-0.809748
C	1.699951	-1.170166	-0.794888
H	2.802589	-1.127985	-0.860922
H	1.343827	-1.077878	-1.829364
C	1.310230	-2.558700	-0.271528
H	1.712575	-3.350171	-0.910627
H	1.684174	-2.737048	0.740089
H	0.219676	-2.695215	-0.247754
Mg	-0.939923	-0.099062	0.319185

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -515.860387111
E_0 = -515.621262
H = -515.606242
G = -515.664118

0 1

C	0.896191	0.925755	0.341201
C	1.652109	-0.072485	-0.570129
C	1.082863	-1.509748	-0.504858
C	1.288915	2.391587	0.061874
H	1.049811	2.688623	-0.967023
H	0.763086	3.088820	0.724292
H	2.361317	2.587329	0.201940
C	3.176048	-0.084915	-0.327057
H	3.682674	-0.790423	-0.995013
H	3.614322	0.900165	-0.501939
H	3.412238	-0.368438	0.703325
C	1.139098	-2.192914	0.867037
H	1.613988	-2.135879	-1.231884
H	0.036899	-1.494788	-0.853582
H	0.705826	-3.195901	0.820211
H	2.167846	-2.296855	1.220481
H	0.589494	-1.631590	1.629283
C	-3.342322	0.479405	0.223871
C	-3.933087	-0.736273	-0.521056
H	-3.747293	1.403960	-0.210661
H	-3.699856	0.477857	1.263058
H	-5.030772	-0.753485	-0.496887
H	-3.643221	-0.750527	-1.577698
H	-3.595603	-1.685405	-0.089931
H	1.503968	0.258896	-1.609039
H	1.178570	0.707111	1.383070
Mg	-1.226848	0.649005	0.263558

Products (Et-Mg-Et)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -514.643847112
E_0 = -514.428479
H = -514.413460
G = -514.470863

0 1

C	-0.963670	0.263673	-0.007190
C	-1.948093	-0.659534	0.011980
C	-1.285905	1.755110	-0.004030
H	-1.881352	2.014621	0.881956
H	-1.910292	2.012165	-0.870579
C	-3.432148	-0.347018	0.038081
H	-3.905632	-0.782195	0.927155
H	-3.641394	0.722116	0.036797
H	-3.938345	-0.790796	-0.828407
C	-1.676589	-2.149480	0.009876
H	-2.101627	-2.636518	0.896472
H	-0.605513	-2.388805	-0.006383
C	3.051966	-1.052723	-0.077833
C	4.143315	0.023491	0.105333
H	3.219560	-1.581293	-1.026528
H	3.168777	-1.823195	0.696918
H	5.158128	-0.394990	0.076309
H	4.098553	0.790386	-0.676021
H	4.047672	0.546034	1.063741
H	-2.129256	-2.639120	-0.861485
C	-0.042848	2.652449	-0.025886
H	0.591031	2.474254	0.851860
H	0.561620	2.471488	-0.923652
H	-0.303569	3.714915	-0.023288
Mg	1.041289	-0.385406	-0.043071

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -514.641756551
E_0 = -514.426412
H = -514.411221
G = -514.469593

0 1

C	0.595826	0.963641	-0.013695
C	1.682136	0.185985	-0.215348
C	0.765631	2.450879	0.274143
H	1.340803	2.964565	-0.507796
H	-0.191987	2.975161	0.349030
H	1.292591	2.628070	1.220862
C	3.111764	0.699877	-0.182511
H	3.748795	0.153260	-0.886197
H	3.171875	1.760930	-0.429898
H	3.559653	0.576472	0.811346
C	1.578093	-1.306268	-0.477042
C	2.198413	-2.190718	0.617935
H	2.059506	-1.545279	-1.435429
H	0.522471	-1.597142	-0.601821
H	2.078705	-3.251669	0.380328
H	3.268302	-1.996355	0.727560
H	1.725294	-2.002146	1.586245
C	-3.230642	-0.806016	-0.198952
C	-4.411314	0.105544	0.198144
H	-3.233670	-1.701650	0.437710
H	-3.391431	-1.185337	-1.217544
H	-5.380189	-0.407271	0.134239
H	-4.318941	0.472558	1.226483
H	-4.482159	0.989211	-0.445924
Mg	-1.292422	0.045757	-0.113770

Products (Et-Mg-Et)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -899.426698479
E_0 = -899.082105
H = -899.060792
G = -899.134822

0 1

C	0.745573	0.549679	-1.009959
C	1.447115	1.526212	-1.975042
C	2.093596	2.754868	-1.320369
H	2.589727	3.385525	-2.064240
H	1.342175	3.382470	-0.822798
H	2.838936	2.480274	-0.570058
C	-1.606632	2.717221	1.826714
C	-2.834217	3.486861	1.296677
H	-0.904344	3.424931	2.287949
H	-1.918813	2.053997	2.644849
H	-3.344698	4.060909	2.081506
H	-2.563056	4.203096	0.512651
H	-3.584437	2.815112	0.863874
H	0.700681	1.881744	-2.694906
H	2.204691	1.012392	-2.590906
C	-0.078720	-0.474958	-1.858298
H	0.585314	-1.245638	-2.275696
H	-0.490294	0.069340	-2.715654
C	-1.231365	-1.151040	-1.146913
C	-2.419046	-0.443623	-0.899138
C	-1.153559	-2.472932	-0.696104
C	-3.481883	-1.026347	-0.208373
H	-2.537735	0.561663	-1.300315
C	-2.213035	-3.061733	-0.006286
H	-0.249575	-3.042495	-0.882028
C	-3.378326	-2.339709	0.247038
H	-4.391569	-0.460807	-0.039358
H	-2.127203	-4.087755	0.334782
H	-4.201430	-2.798497	0.782788
C	1.700840	-0.175421	-0.073787
C	1.223034	-0.813517	1.090526
C	3.088864	-0.255679	-0.294304
C	2.063954	-1.485337	1.974251
H	0.156274	-0.812984	1.309078
C	3.938464	-0.919746	0.589688
H	3.521191	0.205797	-1.173276
C	3.434955	-1.539608	1.730900
H	1.646304	-1.960062	2.855638
H	5.003193	-0.951175	0.382258
H	4.097442	-2.050484	2.420159
Mg	-0.534204	1.551792	0.420865

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -899.432326407
E_0 = -899.087410
H = -899.065995
G = -899.141504

0 1

C	0.409596	-0.474423	-0.543715
C	-0.651068	-1.135114	0.350554
C	-0.741124	-2.669863	0.115032
C	-1.156030	-3.109909	-1.292037
H	-1.450121	-3.086852	0.838010
H	0.235154	-3.112885	0.359188
H	-1.228311	-4.199793	-1.345860
H	-2.131552	-2.698817	-1.562961
H	-0.436206	-2.792413	-2.051767
C	4.456694	-1.699088	-0.053741
C	5.165323	-1.239879	1.237633
H	5.010115	-1.327171	-0.926479
H	4.506379	-2.793481	-0.130913
H	6.210463	-1.573115	1.280812
H	5.178156	-0.149074	1.332452
H	4.674636	-1.629323	2.136331
H	-0.338414	-1.031320	1.397728
H	0.174305	-0.629127	-1.601460
C	0.707827	0.974851	-0.324484
C	1.214361	1.761142	-1.384102
C	0.597211	1.608087	0.931374
C	1.595331	3.086373	-1.200488
H	1.291759	1.320494	-2.375344
C	0.977833	2.936046	1.113318
H	0.191515	1.062514	1.775791
C	1.483769	3.687074	0.053893
H	1.971810	3.655939	-2.043781
H	0.869583	3.389005	2.093374
H	1.776478	4.720240	0.199356
C	-2.048582	-0.507195	0.280469
C	-2.889590	-0.577496	1.398846
C	-2.543498	0.114318	-0.870059
C	-4.181377	-0.057131	1.370163
H	-2.524405	-1.043890	2.309857
C	-3.837032	0.634941	-0.907213
H	-1.910750	0.206881	-1.744659
C	-4.662877	0.550413	0.211322
H	-4.809082	-0.121058	2.252575
H	-4.196423	1.114298	-1.811516
H	-5.666420	0.960050	0.184022
Mg	2.435060	-1.128333	-0.290446

Products (Et-Mg-Et)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -898.214769767
E_0 = -897.893048
H = -897.872941
G = -897.942475

0 1

C	0.099848	1.430569	-0.099137
C	-0.570936	0.251327	-0.022062
C	4.252435	1.162587	-0.803440
C	5.218323	0.672500	0.295468
H	4.507792	2.196192	-1.075941
H	4.423054	0.579795	-1.719246
H	6.272316	0.735760	-0.007043
H	5.122775	1.257687	1.217422
H	5.032347	-0.373266	0.564757
C	-2.059308	0.080555	-0.004580
C	-2.674077	-0.699965	0.987538
C	-2.879715	0.678476	-0.971892
C	-4.056735	-0.857870	1.025093
H	-2.059585	-1.181881	1.740380
C	-4.263662	0.513884	-0.942834
H	-2.425534	1.266225	-1.761092
C	-4.858583	-0.251392	0.058256
H	-4.509133	-1.456731	1.808172
H	-4.876698	0.981445	-1.705816
H	-5.935122	-0.378243	0.082770
C	-0.598687	2.773466	-0.083819
H	-0.644920	3.166833	-1.109385
H	-1.638770	2.693718	0.254823
C	0.129830	3.807660	0.789104
H	0.189999	3.470231	1.828192
H	1.152985	3.981743	0.436085
H	-0.388902	4.770962	0.779745
C	0.218490	-1.021606	0.032018
C	-0.062966	-2.097044	-0.829183
C	1.303572	-1.165568	0.918416
C	0.732924	-3.237068	-0.837618
H	-0.907473	-2.023470	-1.504925
C	2.102833	-2.313804	0.912221
H	1.464901	-0.404219	1.677859
C	1.825560	-3.349149	0.026817
H	0.504810	-4.044115	-1.525439
H	2.924247	-2.401045	1.614694
H	2.440618	-4.241517	0.017726
Mg	2.182951	1.094878	-0.359660

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -898.212937711
E_0 = -897.891237
H = -897.870093
G = -897.944321

0 1

C	0.711276	-0.052000	-0.075192
C	-0.111142	-1.123118	0.010328
C	0.430696	-2.545296	0.013508
C	0.075263	-3.349667	-1.247340
H	0.057723	-3.085523	0.891942
H	1.524183	-2.520567	0.128021
H	0.484156	-4.362595	-1.192970
H	-1.007333	-3.429403	-1.369577
H	0.476676	-2.867272	-2.143426
C	4.918506	-0.412614	-0.217785
C	5.612314	-1.065146	0.996501
H	5.320133	0.598747	-0.367060
H	5.188246	-0.961028	-1.130581
H	6.703805	-1.102911	0.884950
H	5.410849	-0.520960	1.925692
H	5.277785	-2.096152	1.156028
C	0.232830	1.353647	-0.025308
C	0.559965	2.255344	-1.054601
C	-0.471809	1.864177	1.080218
C	0.176658	3.593687	-0.999894
H	1.105420	1.892881	-1.922396
C	-0.842500	3.204616	1.143607
H	-0.728575	1.196376	1.894551
C	-0.525674	4.077647	0.102808
H	0.430827	4.259652	-1.817741
H	-1.384985	3.569264	2.009566
H	-0.817196	5.120572	0.152985
C	-1.607811	-1.034256	0.060983
C	-2.333528	-1.656952	1.087755
C	-2.325326	-0.345196	-0.927071
C	-3.723601	-1.577204	1.136895
H	-1.806019	-2.194095	1.868731
C	-3.715591	-0.273815	-0.886596
H	-1.784952	0.135995	-1.733267
C	-4.421513	-0.886645	0.147441
H	-4.261469	-2.055029	1.948691
H	-4.248284	0.261624	-1.664998
H	-5.503692	-0.828520	0.181201
Mg	2.810718	-0.264526	-0.148158

Products (Ph-Mg-Ph)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -820.784488402
E_0 = -820.494717
H = -820.476273
G = -820.543993

0 1

C	1.637262	-1.241368	0.283880
C	2.030029	-1.842432	1.642034
H	1.501293	-1.391435	2.488582
H	1.796473	-2.911086	1.662429
H	3.103999	-1.740863	1.860445
C	2.152120	-2.120815	-0.880071
H	1.724338	-1.805744	-1.839024
H	1.781715	-3.141233	-0.726501
C	3.684131	-2.171778	-1.033488
H	3.970009	-2.809655	-1.875674
H	4.098875	-1.176083	-1.211838
H	4.163172	-2.575969	-0.137966
C	1.948010	0.222490	0.143571
C	1.870011	0.880921	-1.111660
C	2.237240	1.048818	1.255597
C	2.052236	2.254221	-1.238295
H	1.680482	0.303665	-2.010853
C	2.414755	2.424858	1.124142
H	2.337959	0.607999	2.239176
C	2.322419	3.043746	-0.120284
H	1.988968	2.709048	-2.221345
H	2.638426	3.015466	2.006592
H	2.464413	4.113336	-0.219569
C	-2.488962	-0.303674	0.019126
C	-2.946127	1.025437	-0.089748
C	-3.483245	-1.302163	0.058585
C	-4.304704	1.341061	-0.153803
H	-2.234486	1.847121	-0.126488
C	-4.845093	-1.000317	-0.005407
H	-3.203994	-2.350819	0.141987
C	-5.259203	0.326144	-0.111515
H	-4.617887	2.377116	-0.236651
H	-5.580819	-1.797792	0.028042
H	-6.315839	0.566693	-0.160871
Mg	-0.451865	-0.779222	0.136962

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -820.786906804
E_0 = -820.497308
H = -820.478893
G = -820.546685

0 1

C	1.767274	-1.857921	-0.295907
C	2.722175	-0.839994	0.398019
C	2.186017	0.573274	0.210654
C	2.003236	-3.303963	0.167832
H	1.791646	-3.426363	1.236863
H	1.353307	-4.005049	-0.366060
H	3.034260	-3.651491	0.007643
C	4.196519	-0.964911	-0.035682
H	4.837156	-0.256157	0.498504
H	4.570160	-1.971294	0.166777
H	4.311791	-0.782196	-1.108112
C	-2.234557	-0.513647	-0.068746
C	-3.225023	-1.514436	-0.149299
C	-2.705284	0.810025	0.050288
C	-4.590387	-1.222081	-0.113653
H	-2.938882	-2.560875	-0.243050
C	-4.066771	1.118514	0.085527
H	-1.997841	1.633567	0.117994
C	-5.015218	0.100020	0.003731
H	-5.320415	-2.023181	-0.177830
H	-4.388237	2.151647	0.177060
H	-6.074207	0.334199	0.031402
C	2.235615	1.221762	-1.035020
C	1.552355	1.244248	1.268825
C	1.678401	2.487074	-1.210854
H	2.720705	0.735405	-1.874079
C	0.993025	2.512549	1.095491
H	1.517097	0.774453	2.247786
C	1.054791	3.138965	-0.146317
H	1.733450	2.967550	-2.181649
H	0.516220	3.008849	1.933489
H	0.624077	4.123882	-0.285097
H	2.684739	-1.043572	1.476603
H	1.984829	-1.808583	-1.376255
Mg	-0.189405	-1.011471	-0.135944

Products (Ph-Mg-Ph)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -819.570819699
E_0 = -819.304583
H = -819.286331
G = -819.354127

0 1

C	1.304506	0.875862	0.005500
C	1.733889	2.154654	-0.033124
C	3.187707	2.578938	0.008191
H	3.361804	3.262820	0.847782
H	3.865766	1.732397	0.109424
H	3.459458	3.130391	-0.900220
C	-2.779240	-0.085502	-0.029539
C	-3.600096	0.111908	1.099647
C	-3.413159	-0.621173	-1.169307
C	-4.960502	-0.202573	1.097590
H	-3.180804	0.522297	2.016437
C	-4.772331	-0.940300	-1.186073
H	-2.843497	-0.801366	-2.078955
C	-5.550811	-0.730863	-0.049101
H	-5.558276	-0.036096	1.988272
H	-5.222905	-1.351777	-2.083874
H	-6.607182	-0.977332	-0.056604
C	2.244433	-0.276320	0.042290
C	2.389688	-1.054343	1.204603
C	2.965002	-0.674929	-1.097731
C	3.230412	-2.164933	1.233714
H	1.845473	-0.771410	2.100930
C	3.800521	-1.789915	-1.072451
H	2.862829	-0.099443	-2.011933
C	3.939994	-2.541200	0.093785
H	3.330710	-2.738382	2.149193
H	4.344931	-2.072314	-1.967513
H	4.589035	-3.409260	0.113239
C	0.783551	3.330083	-0.098748
H	0.972047	3.942938	-0.988415
H	-0.269461	3.025357	-0.130493
H	0.908619	3.991320	0.767160
Mg	-0.739994	0.402792	-0.014158

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -819.569834181
E_0 = -819.303488
H = -819.285283
G = -819.351345

0 1

C	1.621793	-1.937431	0.092615
C	2.623807	-1.028066	0.013126
C	1.858378	-3.428923	0.056193
H	1.372875	-3.915138	0.910651
H	1.399143	-3.871248	-0.836583
H	2.910243	-3.736655	0.064365
C	4.107368	-1.308203	-0.149948
H	4.686147	-0.828490	0.647199
H	4.328504	-2.374609	-0.132790
H	4.490540	-0.912199	-1.097033
C	-2.274778	-0.415117	-0.031512
C	-2.727787	0.919901	-0.031122
C	-3.276822	-1.404101	-0.116378
C	-4.082444	1.250431	-0.108458
H	-2.011214	1.736397	0.029354
C	-4.635655	-1.090189	-0.192536
H	-3.004874	-2.458391	-0.123924
C	-5.042434	0.242814	-0.188582
H	-4.389351	2.291994	-0.106262
H	-5.374717	-1.883070	-0.255222
H	-6.096252	0.493814	-0.247854
C	2.264452	0.425501	0.064619
C	2.705215	1.339152	-0.909915
C	1.427624	0.924056	1.084081
C	2.294662	2.667927	-0.890265
H	3.356754	0.996548	-1.705400
C	1.014346	2.260967	1.104423
H	1.175446	0.273514	1.918199
C	1.440738	3.135975	0.111664
H	2.635241	3.344229	-1.666860
H	0.380160	2.614516	1.909799
H	1.125925	4.172941	0.122002
Mg	-0.241278	-0.939360	0.093528

Products (Ph-Mg-Ph)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1204.35276271
E_0 = -1203.957624
H = -1203.932953
G = -1204.015433

0 1

C	1.353998	-0.383421	-0.202481
C	1.244429	-1.768934	-0.903680
H	1.539750	-1.647282	-1.946910
C	2.193940	0.571209	-1.025856
C	3.464572	1.017476	-0.623467
C	1.740092	1.013070	-2.284010
C	4.229575	1.863068	-1.425753
H	3.864692	0.695564	0.330414
C	2.503506	1.849067	-3.093406
H	0.763162	0.694420	-2.641928
C	3.756686	2.286481	-2.665652
H	5.206792	2.184096	-1.080197
H	2.113026	2.169123	-4.053580
H	4.351169	2.946078	-3.287395
C	-2.462564	1.402914	0.160211
C	-2.416466	2.793664	0.387397
C	-3.748487	0.833815	0.067125
C	-3.571550	3.567619	0.516968
H	-1.458434	3.303413	0.468430
C	-4.912366	1.595264	0.193707
H	-3.859430	-0.233750	-0.110017
C	-4.825944	2.967777	0.420700
H	-3.492913	4.636010	0.692899
H	-5.884960	1.118909	0.115853
H	-5.726814	3.563831	0.521145
C	1.685830	-0.414738	1.265885
C	1.916190	-1.592909	2.002534
C	1.708794	0.793699	2.005323
C	2.155183	-1.567089	3.378439
H	1.915654	-2.554770	1.504710
C	1.950498	0.821115	3.372224
H	1.550222	1.733710	1.483574
C	2.175644	-0.364595	4.076209
H	2.329865	-2.501056	3.902534
H	1.959053	1.772607	3.893154
H	2.358162	-0.346755	5.144250
C	-0.141023	-2.398268	-0.897610
C	-0.684017	-2.927368	-2.077173
C	-0.942772	-2.432030	0.259683
C	-1.967256	-3.469368	-2.105094
H	-0.090449	-2.909407	-2.985394
C	-2.231643	-2.975338	0.233251
H	-0.532825	-2.100436	1.210515
C	-2.748735	-3.493926	-0.950134
H	-2.361191	-3.867314	-3.033827
H	-2.821256	-2.998149	1.142897
H	-3.747905	-3.912971	-0.973833
H	1.968247	-2.485539	-0.487900
Mg	-0.708359	0.267513	-0.026787

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1204.35625949
E_0 = -1203.961036
H = -1203.936267
G = -1204.020434

0 1

C	0.570812	0.581991	0.410146
C	1.316389	-0.492095	-0.416864
C	0.593667	-1.823784	-0.206622
C	-3.621865	0.230492	0.066484
C	-4.316757	1.456959	0.023533
C	-4.417390	-0.932784	0.044780
C	-5.710325	1.522719	-0.039559
H	-3.769019	2.397159	0.037976
C	-5.811505	-0.882206	-0.016009
H	-3.947783	-1.913589	0.076619
C	-6.462567	0.349622	-0.059331
H	-6.207762	2.487060	-0.072829
H	-6.389162	-1.801411	-0.029758
H	-7.545410	0.394884	-0.107467
C	0.859969	-2.646598	0.894837
C	-0.440642	-2.202738	-1.078878
C	0.109981	-3.798877	1.122844
H	1.668014	-2.387284	1.569228
C	-1.191319	-3.360307	-0.854163
H	-0.627197	-1.613707	-1.975001
C	-0.920370	-4.159296	0.253625
H	0.334212	-4.422087	1.981651
H	-1.974179	-3.637773	-1.551034
H	-1.497217	-5.059247	0.432469
H	1.192668	-0.254233	-1.479892
H	0.711594	0.362075	1.477108
C	0.902200	2.016111	0.156039
C	0.733985	2.968029	1.182481
C	1.330568	2.502371	-1.092948
C	0.964506	4.323207	0.971920
H	0.417812	2.631272	2.166519
C	1.563339	3.860344	-1.304868
H	1.495721	1.815040	-1.915236
C	1.380498	4.783756	-0.278061
H	0.825693	5.022693	1.789762
H	1.896714	4.195877	-2.281444
H	1.564292	5.838769	-0.444641
C	2.827860	-0.616184	-0.190099
C	3.605174	-1.283838	-1.146381
C	3.470300	-0.101700	0.938073
C	4.977120	-1.444305	-0.976627
H	3.127068	-1.684842	-2.035481
C	4.845612	-0.263235	1.115492
H	2.900882	0.445120	1.679444
C	5.603854	-0.935837	0.161476
H	5.557769	-1.962847	-1.731867
H	5.324031	0.147966	1.997767
H	6.672859	-1.056186	0.296890
Mg	-1.525847	0.178699	0.169276

Products (Ph-Mg-Ph)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1203.14078064
E_0 = -1202.768408
H = -1202.744094
G = -1202.826046

0 1			
C	-0.523569	0.603924	0.138435
C	-1.158803	-0.598155	0.075613
C	3.658597	0.555816	-0.049964
C	4.531446	-0.546200	-0.155113
C	4.265559	1.828595	-0.076850
C	5.914151	-0.394853	-0.278976
H	4.133327	-1.558727	-0.143130
C	5.646763	1.995744	-0.198284
H	3.655950	2.727062	-0.000667
C	6.476383	0.880505	-0.300406
H	6.552098	-1.269785	-0.358878
H	6.074338	2.993514	-0.213621
H	7.549996	1.003963	-0.395668
C	-0.320206	-1.836619	0.153079
C	-0.444066	-2.867453	-0.794926
C	0.669650	-1.978755	1.146115
C	0.413028	-3.961913	-0.778506
H	-1.210819	-2.793200	-1.557443
C	1.529653	-3.083249	1.164613
H	0.699318	-1.264148	1.965595
C	1.409951	-4.072546	0.195331
H	0.309597	-4.733751	-1.533339
H	2.272317	-3.172867	1.949473
H	2.072283	-4.930338	0.204189
C	-2.624754	-0.819212	-0.126313
C	-3.341488	-0.113204	-1.103620
C	-3.318716	-1.758556	0.652448
C	-4.704873	-0.328458	-1.286074
H	-2.823282	0.607135	-1.724339
C	-4.684876	-1.966497	0.479001
H	-2.784161	-2.325305	1.407257
C	-5.384229	-1.252005	-0.492600
H	-5.237381	0.225725	-2.051241
H	-5.202394	-2.688846	1.100906
H	-6.446551	-1.417064	-0.633435
C	-1.225206	1.903572	0.179177
C	-0.870363	2.936096	-0.707596
C	-2.203285	2.190137	1.149609
C	-1.488859	4.182578	-0.655493
H	-0.107155	2.750316	-1.458247
C	-2.806161	3.442830	1.217202
H	-2.486503	1.419070	1.856915
C	-2.459471	4.444752	0.310883
H	-1.205146	4.953445	-1.364042
H	-3.553051	3.637000	1.979734
H	-2.932648	5.418787	0.362217
Mg	1.577695	0.341397	0.122254

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1203.14078064
E_0 = -1202.768408
H = -1202.744094
G = -1202.826046

0 1			
C	-0.523569	0.603924	0.138435
C	-1.158803	-0.598155	0.075613
C	3.658597	0.555816	-0.049964
C	4.531446	-0.546200	-0.155113
C	4.265559	1.828595	-0.076850
C	5.914151	-0.394853	-0.278976
H	4.133327	-1.558727	-0.143130
C	5.646763	1.995744	-0.198284
H	3.655950	2.727062	-0.000667
C	6.476383	0.880505	-0.300406
H	6.552098	-1.269785	-0.358878
H	6.074338	2.993514	-0.213621
H	7.549996	1.003963	-0.395668
C	-0.320206	-1.836619	0.153079
C	-0.444066	-2.867453	-0.794926
C	0.669650	-1.978755	1.146115
C	0.413028	-3.961913	-0.778506
H	-1.210819	-2.793200	-1.557443
C	1.529653	-3.083249	1.164613
H	0.699318	-1.264148	1.965595
C	1.409951	-4.072546	0.195331
H	0.309597	-4.733751	-1.533339
H	2.272317	-3.172867	1.949473
H	2.072283	-4.930338	0.204189
C	-2.624754	-0.819212	-0.126313
C	-3.341488	-0.113204	-1.103620
C	-3.318716	-1.758556	0.652448
C	-4.704873	-0.328458	-1.286074
H	-2.823282	0.607135	-1.724339
C	-4.684876	-1.966497	0.479001
H	-2.784161	-2.325305	1.407257
C	-5.384229	-1.252005	-0.492600
H	-5.237381	0.225725	-2.051241
H	-5.202394	-2.688846	1.100906
H	-6.446551	-1.417064	-0.633435
C	-1.225206	1.903572	0.179177
C	-0.870363	2.936096	-0.707596
C	-2.203285	2.190137	1.149609
C	-1.488859	4.182578	-0.655493
H	-0.107155	2.750316	-1.458247
C	-2.806161	3.442830	1.217202
H	-2.486503	1.419070	1.856915
C	-2.459471	4.444752	0.310883
H	-1.205146	4.953445	-1.364042
H	-3.553051	3.637000	1.979734
H	-2.932648	5.418787	0.362217
Mg	1.577695	0.341397	0.122254

Transition States (Et-Mg-Et)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -515.757569541
E_0 = -515.528244
H = -515.511656
G = -515.573673

0 1

C	-2.756238	0.040987	0.252439
C	-1.664569	-0.603758	-0.334098
H	-3.760570	-0.396844	0.153421
H	-2.217420	0.428202	-0.885104
C	-2.673207	1.249341	1.143881
H	-3.467841	1.966705	0.925134
H	-2.819526	0.912294	2.175990
H	-1.701363	1.739686	1.074326
C	-1.972272	-1.867570	-1.094171
H	-1.520254	-2.687566	-0.525208
H	-3.041543	-2.085362	-1.221438
H	-1.480397	-1.883935	-2.069862
C	1.569500	-1.887455	0.324201
C	3.077119	-1.855862	0.647543
H	1.404527	-2.543944	-0.545648
H	1.037467	-2.390495	1.147871
H	3.507968	-2.850980	0.832590
H	3.657462	-1.410225	-0.168683
H	3.287885	-1.253452	1.538984
C	0.816330	2.122644	-0.237970
C	2.218542	2.658199	-0.598548
H	0.501674	2.590617	0.710318
H	0.092319	2.500824	-0.979136
H	2.269130	3.755150	-0.659683
H	2.969900	2.350172	0.137519
H	2.561820	2.275336	-1.566968
Mg	0.585628	-0.012945	-0.057840

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -515.801156847
E_0 = -515.566227
H = -515.550941
G = -515.607489

0 1

C	1.616345	-1.044069	-0.159193
C	1.713864	0.360163	-0.399501
H	1.704689	-1.658709	-1.057612
H	2.228378	0.949589	0.355543
C	2.224033	-1.651951	1.100705
H	1.846558	-2.661020	1.289540
H	3.319783	-1.726960	1.041708
H	1.998167	-1.058040	1.992649
C	1.921223	0.847854	-1.816084
H	2.961423	0.654271	-2.105079
H	1.290581	0.305815	-2.528090
H	1.726939	1.914585	-1.932737
C	-2.515128	-1.169978	-0.244530
C	-3.576840	-0.065601	-0.414543
H	-2.746131	-1.763431	0.650956
H	-2.589250	-1.881875	-1.077840
H	-4.600471	-0.462141	-0.457467
H	-3.556236	0.655715	0.410578
H	-3.425581	0.509371	-1.335395
C	0.005701	1.670535	0.201992
C	-0.212955	1.604395	1.716710
H	-0.782609	2.457077	2.106426
H	0.742193	1.579663	2.250702
H	-0.774452	0.713279	2.047294
H	0.629123	2.518422	-0.068601
H	-0.947210	1.812060	-0.337843
Mg	-0.506946	-0.513813	-0.096506

Transition States (Et-Mg-Et)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -514.524981637
E_0 = -514.316440
H = -514.299825
G = -514.361725

0 1

C	2.404418	-0.477963	-0.069539
C	1.174031	-0.287467	0.041167
C	3.858429	-0.405164	-0.207263
H	4.214743	-0.988358	-1.060428
H	4.127148	0.641499	-0.368545
H	4.364229	-0.751836	0.697694
C	-1.189703	2.480364	0.060101
C	0.131605	3.275163	0.029264
H	-1.761464	2.773020	0.953905
H	-1.820544	2.801750	-0.782304
H	-0.010395	4.365796	0.056295
H	0.777480	3.024812	0.880212
H	0.714428	3.061144	-0.875687
C	-2.091870	-1.538974	-0.054595
C	-3.632967	-1.512540	-0.125009
H	-1.790337	-2.139168	0.820564
H	-1.712682	-2.110884	-0.919486
H	-4.091771	-2.511514	-0.161792
H	-4.067253	-1.000422	0.741579
H	-3.987797	-0.972311	-1.010478
C	1.538855	-2.050174	0.288053
H	1.445772	-2.226305	1.354652
H	0.661043	-2.383197	-0.258203
H	2.399584	-2.586115	-0.119008
Mg	-1.051580	0.341884	0.023163

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -514.563820123
E_0 = -514.352246
H = -514.336896
G = -514.394985

0 1

C	1.404290	-1.184231	0.061558
C	1.713314	0.012383	-0.201999
C	2.114781	-2.478114	0.321454
H	1.828815	-3.225458	-0.423591
H	3.205709	-2.373182	0.300544
H	1.827413	-2.885147	1.294391
C	2.765996	1.015703	-0.455328
H	3.732424	0.535612	-0.258548
H	2.760783	1.360065	-1.491876
H	2.682698	1.888447	0.194333
C	-2.598180	-1.151483	0.143098
C	-3.720841	-0.192895	-0.299343
H	-2.749773	-1.432252	1.194531
H	-2.679532	-2.094859	-0.413756
H	-4.724460	-0.618340	-0.160126
H	-3.700997	0.749254	0.260401
H	-3.639122	0.072692	-1.359747
C	-0.021487	1.691389	-0.434154
C	-0.076879	2.486639	0.873090
H	-0.341056	3.541276	0.716393
H	0.883760	2.474809	1.398486
H	-0.819702	2.083809	1.572131
H	0.642907	2.146132	-1.164743
H	-1.017654	1.697341	-0.915127
Mg	-0.614849	-0.426379	-0.066162

Transition States (Et-Mg-Et)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -899.325224097
E_0 = -898.989554
H = -898.967028
G = -899.044774

0 1

C	-0.277319	-1.617251	-0.260543
C	0.596390	-0.524366	-0.084130
H	0.139633	-2.625820	-0.372178
H	0.087736	-0.884831	-1.255697
C	-0.262404	2.302336	2.101953
C	-1.308785	3.409932	2.348044
H	0.702435	2.632327	2.518245
H	-0.524111	1.418671	2.703938
H	-1.418261	3.681853	3.408317
H	-1.056269	4.332406	1.812783
H	-2.307120	3.117242	1.998422
C	0.226927	2.530331	-1.955353
C	-0.199121	4.000134	-2.148597
H	-0.389895	1.890106	-2.606599
H	1.250683	2.404345	-2.342569
H	-0.134298	4.341838	-3.192203
H	-1.233941	4.167915	-1.828085
H	0.421041	4.682767	-1.556143
C	2.034023	-0.855273	-0.006002
C	2.492057	-1.882567	0.838983
C	2.982833	-0.087659	-0.705475
C	3.853716	-2.135600	0.975018
H	1.779346	-2.460084	1.418045
C	4.340531	-0.368188	-0.594830
H	2.644253	0.717145	-1.349149
C	4.780629	-1.387663	0.250095
H	4.191887	-2.917260	1.646004
H	5.057884	0.219116	-1.156648
H	5.840705	-1.590370	0.351251
C	-1.756526	-1.572462	-0.190775
C	-2.435399	-0.554776	0.493870
C	-2.495001	-2.596378	-0.802943
C	-3.826403	-0.550385	0.538402
H	-1.875954	0.208601	1.023881
C	-3.884731	-2.586820	-0.760564
H	-1.975160	-3.397756	-1.318244
C	-4.552532	-1.559872	-0.092878
H	-4.342563	0.235882	1.076752
H	-4.446299	-3.378311	-1.243054
H	-5.635908	-1.553260	-0.054790
Mg	0.114239	1.748054	0.054339

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -899.379366385
E_0 = -899.038187
H = -899.016839
G = -899.089641

0 1

C	-0.192133	-0.910775	-0.665635
C	0.763814	-0.581812	0.351313
H	0.156359	-1.074177	-1.678468
H	0.614190	-1.054134	1.318360
C	-1.748721	2.865667	-1.186730
C	-2.099370	4.017062	-0.222349
H	-2.650443	2.556928	-1.731510
H	-1.063114	3.237709	-1.960667
H	-2.516317	4.891636	-0.739893
H	-2.841773	3.712700	0.524253
H	-1.222661	4.371953	0.331961
C	0.609666	1.326122	1.440658
C	1.095557	0.860400	2.801503
H	1.262714	1.698079	3.488027
H	2.041382	0.318481	2.723023
H	0.369773	0.194469	3.282878
H	1.350224	1.946772	0.928290
H	-0.285276	1.956875	1.608818
C	-1.565811	-1.248772	-0.343423
C	-2.115320	-1.022623	0.948952
C	-2.458797	-1.730079	-1.339730
C	-3.466012	-1.274049	1.216512
H	-1.473315	-0.711451	1.766520
C	-3.788760	-1.979502	-1.057628
H	-2.075125	-1.912460	-2.338350
C	-4.311664	-1.749587	0.224581
H	-3.846329	-1.102390	2.217953
H	-4.435903	-2.358391	-1.841646
H	-5.356099	-1.945131	0.435260
C	2.195977	-0.507536	-0.041169
C	3.156675	-1.210560	0.698638
C	2.626650	0.219521	-1.161282
C	4.500181	-1.196901	0.328213
H	2.844570	-1.789014	1.561396
C	3.967646	0.237940	-1.530587
H	1.909029	0.782021	-1.749740
C	4.911610	-0.471015	-0.786769
H	5.223853	-1.755035	0.911756
H	4.278344	0.810343	-2.397561
H	5.956780	-0.454569	-1.073892
Mg	-0.893999	1.151482	-0.303098

Transition States (Et-Mg-Et)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -898.103464019
E_0 = -897.788529
H = -897.766212
G = -897.844556

0 1

C	-0.723862	-0.295717	-0.040627
C	0.534486	-0.298914	0.060842
C	2.482384	-3.245599	0.567888
H	2.977528	-3.368001	1.543190
H	3.097785	-3.832091	-0.130645
C	4.048702	0.352128	-0.610768
H	3.981387	1.183140	0.109366
H	3.694008	0.787707	-1.558488
C	1.072854	-3.860474	0.639068
H	1.068297	-4.920560	0.934170
H	0.437999	-3.333450	1.362475
H	0.558461	-3.806898	-0.329342
C	5.528594	-0.053654	-0.770611
H	6.181928	0.775679	-1.080535
H	5.945094	-0.446235	0.164683
H	5.654068	-0.845830	-1.518362
C	-2.130241	-0.544925	-0.158295
C	-3.064604	0.481992	-0.358176
C	-2.566136	-1.880933	-0.079072
C	-4.415675	0.173978	-0.478952
H	-2.729085	1.509697	-0.413692
C	-3.918344	-2.172692	-0.208072
H	-1.843380	-2.671567	0.081032
C	-4.846210	-1.149753	-0.406740
H	-5.133393	0.971838	-0.630339
H	-4.248363	-3.203294	-0.148532
H	-5.900035	-1.384086	-0.502299
C	-0.109310	3.236047	1.579308
C	0.009128	4.048540	0.449845
C	0.169848	3.476662	-0.813969
C	0.213433	2.095265	-0.953556
C	0.110351	1.271013	0.182031
C	-0.062992	1.853601	1.450919
H	-0.233937	3.681844	2.559284
H	-0.021447	5.126963	0.554666
H	0.265492	4.109076	-1.688813
H	0.348042	1.640284	-1.927116
H	-0.148247	1.212819	2.320227
Mg	2.671114	-1.175536	-0.000608

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -898.133368254
E_0 = -897.815853
H = -897.794476
G = -897.869635

0 1

C	0.689322	-0.059005	-0.165457
C	-0.552159	0.226014	-0.193907
C	-1.212735	2.576170	-0.493647
C	-1.863376	3.086851	0.788638
H	-1.936953	2.164005	-1.190366
H	-0.725995	3.413635	-1.030900
H	-2.635560	3.842860	0.590546
H	-2.352354	2.277426	1.338869
H	-1.138392	3.550737	1.467405
C	2.515738	3.517775	-0.150005
C	3.940411	3.027822	0.169322
H	2.211892	4.271585	0.589967
H	2.519683	4.053310	-1.110247
H	4.675163	3.844292	0.198070
H	3.991597	2.526255	1.142315
H	4.300762	2.308675	-0.574879
C	-1.931080	-0.190190	-0.091488
C	-2.482933	-0.480223	1.168262
C	-2.721597	-0.380927	-1.238676
C	-3.786792	-0.956721	1.274405
H	-1.876818	-0.341988	2.055626
C	-4.021712	-0.858738	-1.125946
H	-2.303040	-0.160343	-2.213600
C	-4.559501	-1.145700	0.130045
H	-4.198562	-1.180507	2.252038
H	-4.618162	-1.009122	-2.018758
H	-5.575188	-1.515111	0.214256
C	1.483580	-1.288888	-0.070936
C	2.869914	-1.222066	0.134858
C	0.888191	-2.558344	-0.189129
C	3.636296	-2.381088	0.231617
H	3.343770	-0.250609	0.220030
C	1.655709	-3.714685	-0.102494
H	-0.180847	-2.630939	-0.351614
C	3.032638	-3.631136	0.111450
H	4.705589	-2.306789	0.395457
H	1.179500	-4.684408	-0.198982
H	3.628806	-4.534081	0.181066
Mg	0.958802	2.079966	-0.256479

Transition States (Ph-Mg-Ph)

(1,1)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -820.690252622
E_0 = -820.408459
H = -820.388933
G = -820.459672

0 1

C	0.743169	3.157192	0.536855
C	0.050994	2.348873	-0.366514
H	0.701419	4.249555	0.419758
H	1.324084	2.528562	-0.475441
C	1.472849	2.673723	1.758027
H	2.415303	3.207411	1.900138
H	0.843014	2.891587	2.627709
H	1.663706	1.599901	1.724145
C	-0.702390	3.063206	-1.459722
H	-1.767334	2.881588	-1.277618
H	-0.540744	4.148629	-1.499318
H	-0.495400	2.632096	-2.442485
C	1.881216	-0.744989	-0.138522
C	2.214208	-1.931774	0.549663
C	2.960206	-0.110022	-0.788824
C	3.514184	-2.441291	0.596171
H	1.437963	-2.488471	1.071812
C	4.267370	-0.604016	-0.760815
H	2.789993	0.804625	-1.360861
C	4.548629	-1.776305	-0.061211
H	3.720757	-3.357343	1.141813
H	5.062222	-0.081282	-1.285256
H	5.559882	-2.168382	-0.031707
C	-2.145645	-0.533223	-0.045364
C	-3.166107	0.352573	0.358996
C	-2.571092	-1.845828	-0.341870
C	-4.506272	-0.029304	0.463212
H	-2.920747	1.384173	0.612278
C	-3.905926	-2.247107	-0.248277
H	-1.843749	-2.591569	-0.658265
C	-4.880982	-1.336440	0.156589
H	-5.256278	0.688579	0.782894
H	-4.185692	-3.268588	-0.488939
H	-5.919394	-1.641835	0.232948
Mg	-0.102956	0.050763	-0.186997

(1,2)-*trans*-2-butene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -820.728943695
E_0 = -820.442273
H = -820.423765
G = -820.490777

0 1

C	1.110158	2.591739	-0.119736
C	2.078501	1.733583	0.486360
H	0.580266	3.226235	0.595532
H	2.996509	1.564108	-0.068973
C	1.409077	3.259421	-1.459491
H	0.500620	3.622176	-1.948712
H	2.081371	4.122913	-1.354870
H	1.890983	2.569434	-2.159695
C	2.272087	1.771352	1.984341
H	2.766513	2.715565	2.240639
H	1.320029	1.755720	2.524558
H	2.891452	0.953107	2.350726
C	1.768970	-0.382869	0.163227
C	2.002926	-0.750124	-1.173437
C	1.978122	-1.366964	1.144322
C	2.399118	-2.042663	-1.527871
H	1.893076	-0.011322	-1.968927
C	2.385594	-2.657194	0.805812
H	1.812772	-1.136451	2.193654
C	2.596587	-2.996693	-0.532422
H	2.565786	-2.298361	-2.569239
H	2.535060	-3.401387	1.581703
H	2.915960	-3.999213	-0.794878
C	-2.118550	0.126756	-0.007179
C	-3.201165	1.028520	-0.045051
C	-2.454776	-1.239386	0.078301
C	-4.530667	0.602621	-0.000588
H	-3.016241	2.098999	-0.111210
C	-3.779167	-1.680918	0.122538
H	-1.669075	-1.991349	0.111889
C	-4.823026	-0.757751	0.083145
H	-5.336586	1.329657	-0.031757
H	-3.996753	-2.742742	0.187794
H	-5.853727	-1.094987	0.117266
Mg	-0.120062	0.773442	-0.075761

Transition States (Ph-Mg-Ph)

(1,1)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -819.457269981
E_0 = -819.196292
H = -819.176710
G = -819.248335

0 1

C	0.273863	3.357554	-0.051219
C	0.171992	2.117073	0.045465
C	0.135625	4.795933	-0.269364
H	0.959455	5.195461	-0.866399
H	-0.797899	4.965820	-0.811178
H	0.084794	5.339520	0.677598
C	1.680372	2.655177	0.895721
H	1.462148	2.668557	1.958753
H	2.232759	1.764972	0.598282
H	2.281894	3.518340	0.603680
C	1.834223	-0.923740	-0.060511
C	2.824181	-0.420292	-0.932613
C	2.262989	-1.961523	0.794552
C	4.135707	-0.904281	-0.957152
H	2.573629	0.374218	-1.636938
C	3.569672	-2.456240	0.790108
H	1.559349	-2.412315	1.492483
C	4.513780	-1.927019	-0.089034
H	4.858490	-0.489798	-1.654260
H	3.850919	-3.256671	1.468218
H	5.529001	-2.309761	-0.100377
C	-2.218098	-0.628482	-0.055308
C	-2.687871	-1.944575	-0.250446
C	-3.217234	0.346820	0.144959
C	-4.046577	-2.268923	-0.247292
H	-1.977906	-2.753758	-0.412610
C	-4.580973	0.042566	0.152214
H	-2.932897	1.386267	0.304825
C	-5.000375	-1.272172	-0.044923
H	-4.361872	-3.296688	-0.401949
H	-5.315319	0.827171	0.311376
H	-6.057517	-1.517196	-0.040991
Mg	-0.154722	-0.137617	-0.056787

(1,2)-2-butyne

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -819.493678061
E_0 = -819.230491
H = -819.211895
G = -819.280469

0 1

C	0.172999	3.997834	0.000721
C	0.651233	2.577435	0.000232
C	1.755829	1.967817	-0.000408
C	3.232638	2.006354	-0.001359
H	3.656473	1.525442	-0.883947
H	3.526407	3.064163	-0.001518
H	3.657646	1.525373	0.880626
C	1.716013	-0.349667	-0.000042
C	2.155679	-0.939980	1.199691
C	2.970118	-2.073369	1.207065
C	3.380704	-2.641252	0.000721
C	2.969925	-2.074305	-1.206002
C	2.155480	-0.940919	-1.199389
H	1.861938	-0.513619	-2.156729
H	3.285792	-2.513794	-2.146899
H	4.018169	-3.518765	0.001011
H	3.286142	-2.512116	2.148255
H	1.862331	-0.511903	2.156746
C	-2.231217	-0.113273	-0.000158
C	-2.517159	-1.493498	-0.000936
C	-3.824357	-1.985894	-0.000986
C	-4.901847	-1.101569	-0.000243
C	-4.659702	0.271216	0.000540
C	-3.346822	0.748074	0.000572
H	-3.201909	1.826595	0.001178
H	-5.492098	0.968592	0.001123
H	-5.919466	-1.477988	-0.000272
H	-4.001904	-3.057137	-0.001599
H	-1.704436	-2.216974	-0.001510
H	0.997215	4.719481	0.000060
H	-0.452636	4.190392	-0.874654
H	-0.451099	4.190254	0.877227
Mg	-0.250471	0.598498	0.000066

Transition States (Ph-Mg-Ph)

(1,1)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1204.25535567
E_0 = -1203.867514
H = -1203.841872
G = -1203.928988

0 1

C	-1.088183	0.586247	-1.911278
C	-0.290622	1.042558	-0.848051
H	-1.573696	1.311004	-2.574518
H	-1.541809	0.680732	-0.686300
C	-1.221046	-0.580073	2.095685
C	-1.469993	-1.805959	2.749804
C	-2.220610	0.402611	2.264645
C	-2.620965	-2.040959	3.505474
H	-0.745454	-2.615261	2.675662
C	-3.378374	0.188832	3.018711
H	-2.097600	1.387356	1.812531
C	-3.583070	-1.040609	3.641947
H	-2.767373	-3.001873	3.990277
H	-4.114891	0.980253	3.125444
H	-4.477921	-1.215970	4.230082
C	2.568833	-0.762670	0.694437
C	3.321933	-0.481688	-0.464994
C	3.272788	-1.424562	1.723442
C	4.668892	-0.830432	-0.598610
H	2.853072	0.028896	-1.306472
C	4.618902	-1.780341	1.610734
H	2.762970	-1.675156	2.652091
C	5.323280	-1.483574	0.444393
H	5.206681	-0.593265	-1.512166
H	5.118703	-2.287981	2.430595
H	6.368979	-1.757554	0.349989
C	-0.166243	2.511847	-0.679690
C	1.088287	3.004682	-0.284037
C	-1.209805	3.431062	-0.891451
C	1.305623	4.374413	-0.154021
H	1.900236	2.309157	-0.098653
C	-0.998728	4.795252	-0.725229
H	-2.202338	3.080353	-1.155259
C	0.262911	5.272717	-0.367881
H	2.286524	4.735600	0.132726
H	-1.819868	5.487870	-0.871846
H	0.425943	6.337095	-0.243784
C	-1.273415	-0.825238	-2.314458
C	-2.410871	-1.174672	-3.057298
C	-0.328357	-1.813531	-2.004571
C	-2.619043	-2.491779	-3.450543
H	-3.137798	-0.411860	-3.316900
C	-0.536451	-3.129506	-2.404157
H	0.589333	-1.550146	-1.490391
C	-1.683326	-3.471963	-3.119993
H	-3.506260	-2.753775	-4.014988
H	0.203746	-3.884313	-2.166292
H	-1.841601	-4.498397	-3.430516
Mg	0.509695	-0.244063	0.885885

(1,2)-*E*-stilbene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1204.30740315
E_0 = -1203.914836
H = -1203.890226
G = -1203.971873

0 1

C	-0.365386	1.723665	-0.657177
C	-1.458286	1.129183	0.047217
H	-0.419559	1.820901	-1.733532
H	-1.679280	1.558206	1.021498
C	-1.111044	-0.687553	1.048195
C	-1.361328	-0.667565	2.428346
C	-1.334986	-1.893119	0.363659
C	-1.779241	-1.809804	3.107963
H	-1.238267	0.255549	2.992760
C	-1.746919	-3.046235	1.034774
H	-1.206862	-1.943111	-0.716490
C	-1.970015	-3.003989	2.409535
H	-1.957486	-1.773020	4.177778
H	-1.907281	-3.967471	0.484599
H	-2.301812	-3.893004	2.934228
C	2.482722	-1.193448	-0.515199
C	3.624188	-0.603106	-1.094820
C	2.510052	-2.596502	-0.389289
C	4.718753	-1.357402	-1.523374
H	3.673470	0.476495	-1.218436
C	3.597985	-3.364496	-0.811703
H	1.663589	-3.119137	0.052042
C	4.708112	-2.744325	-1.382363
H	5.579514	-0.864204	-1.965056
H	3.580068	-4.444036	-0.695400
H	5.556153	-3.335060	-1.712802
C	0.730336	2.375429	0.024065
C	1.716706	3.104681	-0.700508
C	0.950419	2.231149	1.424848
C	2.811888	3.660178	-0.069963
H	1.586476	3.230815	-1.770202
C	2.071130	2.798375	2.046902
H	0.203277	1.750452	2.047381
C	3.007166	3.509584	1.313663
H	3.533496	4.220126	-0.655358
H	2.195540	2.679487	3.117885
H	3.874107	3.943578	1.796495
C	-2.693801	0.771887	-0.702774
C	-3.938401	0.893897	-0.070186
C	-2.666059	0.334778	-2.034604
C	-5.118923	0.603545	-0.747916
H	-3.979044	1.220205	0.963737
C	-3.844989	0.037018	-2.711637
H	-1.718653	0.221594	-2.548948
C	-5.077074	0.171414	-2.072313
H	-6.071194	0.712479	-0.240999
H	-3.801807	-0.300280	-3.741310
H	-5.994626	-0.059948	-2.601240
Mg	0.837681	-0.054505	0.118277

Transition States (Ph-Mg-Ph)

(1,1)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1203.03503874
E_0 = -1202.667613
H = -1202.642258
G = -1202.729503

0 1

C	1.559593	-0.547976	-0.031724
C	0.311640	-0.415086	0.091745
C	2.978191	-0.474874	-0.200510
C	3.537636	0.801934	-0.399749
C	3.804771	-1.607504	-0.172722
C	4.911020	0.927696	-0.566621
H	2.895613	1.674761	-0.418057
C	5.177535	-1.462292	-0.342715
H	3.369842	-2.586857	-0.019851
C	5.733446	-0.199255	-0.539199
H	5.339160	1.911425	-0.719438
H	5.813643	-2.339430	-0.321226
H	6.803880	-0.092320	-0.670731
C	0.231965	-4.185848	-0.860801
C	0.295671	-4.793497	0.394754
C	0.477056	-4.019620	1.542725
C	0.592431	-2.638622	1.440956
C	0.510280	-2.019949	0.180938
C	0.345362	-2.805672	-0.973411
H	0.091094	-4.788305	-1.750457
H	0.203750	-5.870243	0.478722
H	0.526277	-4.493409	2.516114
H	0.728514	-2.027173	2.324636
H	0.289565	-2.322196	-1.941010
C	-3.372909	0.025676	-0.079061
C	-3.524353	-1.374704	-0.159540
C	-4.574479	0.765075	-0.113761
C	-4.771254	-1.996278	-0.267664
H	-2.644701	-2.015832	-0.135735
C	-5.830395	0.162827	-0.221898
H	-4.542429	1.851666	-0.052778
C	-5.932404	-1.225455	-0.300033
H	-4.838635	-3.079135	-0.325582
H	-6.727914	0.774141	-0.244584
H	-6.904498	-1.700532	-0.384022
C	-0.585222	2.925601	0.178406
C	-1.087491	4.038927	-0.527690
C	0.566933	3.174978	0.953421
C	-0.489301	5.300801	-0.474774
H	-1.977589	3.931788	-1.145382
C	1.176115	4.431119	1.026257
H	1.011157	2.368805	1.537158
C	0.648225	5.501744	0.305838
H	-0.911786	6.127520	-1.038538
H	2.055675	4.577108	1.647385
H	1.114207	6.480484	0.355629
Mg	-1.486266	0.989937	0.084062

(1,2)-diphenylacetylene

B3LYP/6-311++G(d,p) optimized geometry (Å).

E = -1203.06101907
E_0 = -1202.692040
H = -1202.667349
G = -1202.751143

0 1

C	-0.162272	1.232371	0.179797
C	-1.121949	0.421758	0.011490
C	-0.590418	-1.840152	0.319678
C	-1.035387	-2.776817	-0.631171
C	-1.549174	-4.014353	-0.249930
C	-1.643655	-4.344874	1.104475
C	-1.220303	-3.434545	2.070434
C	-0.710651	-2.194560	1.675604
H	-0.408996	-1.492444	2.452629
H	-1.293569	-3.684984	3.124025
H	-2.049444	-5.305584	1.402407
H	-1.877427	-4.723550	-1.003245
H	-0.990568	-2.540102	-1.691593
C	3.200923	-0.823520	-0.201924
C	3.708050	-2.090431	-0.555141
C	5.072969	-2.323999	-0.738851
C	5.986406	-1.285049	-0.568643
C	5.523525	-0.018698	-0.214813
C	4.155375	0.200045	-0.037841
H	3.837050	1.201945	0.242113
H	6.227136	0.796603	-0.075885
H	7.047937	-1.460779	-0.708156
H	5.423113	-3.314941	-1.011675
H	3.029351	-2.929941	-0.691939
C	0.026610	2.676673	0.297440
C	1.181211	3.293355	-0.209470
C	-0.936149	3.479162	0.935924
C	1.354648	4.671034	-0.109159
H	1.939821	2.686963	-0.691567
C	-0.747096	4.852022	1.055471
H	-1.828832	3.016476	1.340273
C	0.395158	5.455630	0.528522
H	2.247717	5.129887	-0.518577
H	-1.497710	5.454274	1.555599
H	0.537453	6.526481	0.618672
C	-2.489206	0.165176	-0.387589
C	-3.460361	-0.272355	0.527528
C	-2.873000	0.443992	-1.710119
C	-4.783655	-0.413812	0.129701
H	-3.166426	-0.508265	1.542487
C	-4.198988	0.290611	-2.104375
H	-2.127820	0.786916	-2.417963
C	-5.156755	-0.137574	-1.187147
H	-5.526748	-0.746228	0.845596
H	-4.483664	0.508825	-3.127446
H	-6.189162	-0.257262	-1.495451
Mg	1.132971	-0.534236	0.060862