

**The Products of the Reactions of  $\alpha$ -Benzynes with Ethene, Propene, and Acetylene:  
A Combined Mass Spectrometric and Quantum Chemical Study**

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**Supplement**

Tables of energies and structures of reactants, transition states, intermediates, and products. Energies are given in Hartree ( $E_h$ ), and Cartesian coordinates in Ångström (Å).

## REACTANTS

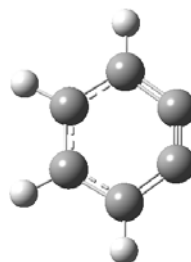
### **C<sub>6</sub>H<sub>4</sub> ( $\sigma$ -Benzyne)**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.074890

Electronic energy (including ZP) E = -230.897795

C	0.000000	0.702713	1.056666
C	0.000000	-0.702713	1.056666
C	0.000000	-1.459308	-0.133940
C	0.000000	-0.622194	-1.234437
C	0.000000	0.622194	-1.234437
C	0.000000	1.459308	-0.133940
H	0.000000	1.227056	2.007018
H	0.000000	-1.227056	2.007018
H	0.000000	-2.541411	-0.136755
H	0.000000	2.541411	-0.136755



### **C<sub>2</sub>H<sub>4</sub> (Ethene)**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.050782

Electronic energy (including ZP) E = -78.564730

C	0.000000	0.000000	0.664389
H	0.000000	0.922841	1.235170
H	0.000000	-0.922841	1.235170
C	0.000000	0.000000	-0.664389
H	0.000000	-0.922841	-1.235170
H	0.000000	0.922841	-1.235170



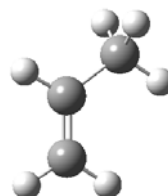
### **C<sub>3</sub>H<sub>6</sub> (Propene)**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.079286

Electronic energy (including ZP) E = -117.866302

C	0.000000	0.472778	0.000000
H	0.277272	1.525954	0.000000
C	-1.291777	0.151513	0.000000
H	-2.066396	0.910172	0.000000
H	-1.620530	-0.883905	0.000000
C	1.137744	-0.505325	0.000000
H	1.777013	-0.364085	0.878717
H	0.779822	-1.537845	0.000000
H	1.777013	-0.364085	-0.878717



### **C<sub>2</sub>H<sub>2</sub> (Acetylene)**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.027031

Electronic energy (including ZP) E = -77.329615

C	0.000000	0.000000	0.599684
H	0.000000	0.000000	1.662817
C	0.000000	0.000000	-0.599684
H	0.000000	0.000000	-1.662817



## INTERMEDIATES & TRANSITION STATES

### Intermediates ( $\sigma$ -C<sub>6</sub>H<sub>4</sub> + C<sub>2</sub>H<sub>4</sub>)

#### C<sub>8</sub>H<sub>8</sub> 'edge-on'

B3LYP/6-311+G(d,p)

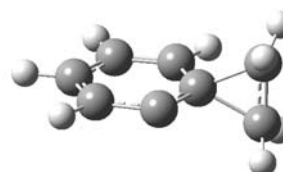
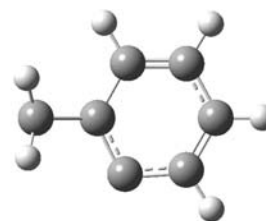
Zero-point correction

ZP = 0.131004

Electronic energy (including ZP)

E = -309.461894

C	0.082146	1.219990	-0.000030
C	1.437107	-1.243317	0.000016
C	2.121194	-0.041855	-0.000011
C	1.444844	1.210971	0.000007
H	-0.467183	2.158342	-0.000030
H	2.023559	-2.159996	0.000004
H	3.209258	-0.037029	-0.000031
H	2.011678	2.134576	0.000085
H	-2.265707	0.875940	-1.258181
H	-2.234078	-0.965493	-1.247480
C	0.015948	-1.340608	0.000070
C	-0.621969	-0.045960	-0.000081
C	-2.054420	-0.039444	-0.720647
C	-2.054503	-0.039336	0.720669
H	-2.265459	0.876266	1.257939
H	-2.234155	-0.965245	1.247742



#### C<sub>8</sub>H<sub>8</sub> 'biradical'

B3LYP/6-311+G(d,p)

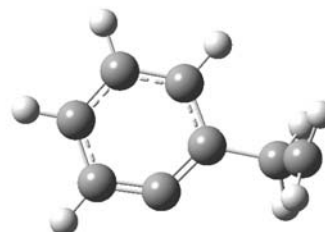
Zero-point correction

ZP = 0.128249

Electronic energy (including ZP)

E = -309.473949

C	0.554179	0.215330	-0.001820
C	-0.457560	1.065677	0.376957
C	0.266063	-1.154248	0.138510
C	-0.966661	-1.580923	0.631755
C	-1.945507	-0.658104	1.001830
C	-1.687275	0.714981	0.878518
H	1.022382	-1.885046	-0.134834
H	-1.162740	-2.642414	0.733263
H	-2.902455	-0.995755	1.385331
H	-2.429298	1.452230	1.165011
C	1.864441	0.820568	-2.053500
C	1.894232	0.700150	-0.565306
H	1.386941	1.672863	-2.521674
H	2.127379	-0.020884	-2.683096
H	2.126716	1.667060	-0.110388
H	2.672644	-0.003375	-0.255495



## Transition States ( $o\text{-C}_6\text{H}_4 + \text{C}_2\text{H}_4$ )

### $\text{C}_8\text{H}_8$ # 'edge-on #1'

B3LYP/6-311+G(d,p)

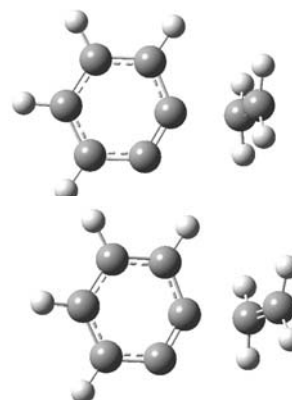
Zero-point correction

ZP = 0.127771

Electronic energy (including ZP)

E = -309.441414

C	0.410320	-0.131126	-0.140110
C	-0.111703	1.162546	-0.095697
C	-1.499286	1.220341	0.019934
C	-2.257196	0.039796	0.095441
C	-1.643596	-1.217408	0.053736
C	-0.245095	-1.254798	0.010034
H	0.487382	2.061141	-0.208788
H	-1.995957	2.184330	0.036008
H	-3.334901	0.109528	0.215301
H	-2.251087	-2.115533	0.122513
C	2.657770	0.054652	0.653335
H	2.770261	1.065701	1.026057
H	2.789332	-0.749966	1.365968
C	2.191914	-0.197501	-0.623818
H	2.270010	-1.199539	-1.021231
H	2.246187	0.585326	-1.372956



### $\text{C}_8\text{H}_8$ # 'edge-on #2'

B3LYP/6-311+G(d,p)

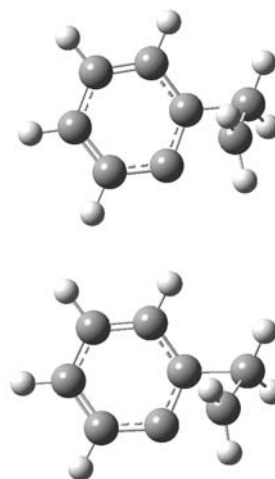
Zero-point correction

ZP = 0.130255

Electronic energy (including ZP)

E = -309.449784

C	-0.214732	1.319794	-0.011051
C	-1.224342	-1.303126	-0.068195
C	-2.069638	-0.227099	0.067672
C	-1.556101	1.103265	0.112993
H	0.206703	2.314339	0.102613
H	-1.641251	-2.305697	-0.006344
H	-3.142073	-0.374018	0.167227
H	-2.235047	1.932623	0.279530
H	1.644526	0.038816	1.734328
H	2.051468	-1.519050	0.839080
C	0.158375	-1.150100	-0.419998
C	0.626260	0.194467	-0.339391
C	1.816515	-0.469664	0.793896
C	2.130170	0.330484	-0.410755
H	2.507782	1.336115	-0.248497
H	2.608860	-0.211250	-1.218968



### $\text{C}_8\text{H}_8$ # 'H-transfer #'

B3LYP/6-311+G(d,p)

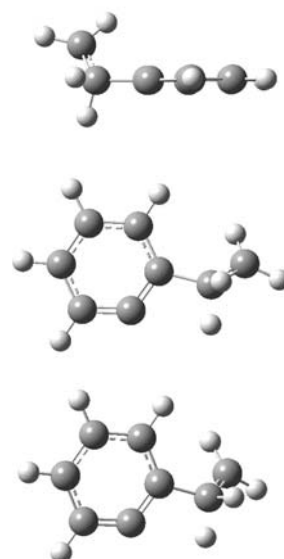
Zero-point correction

ZP = 0.126556

Electronic energy (including ZP)

E = -309.430648

C	-0.041677	-0.014536	0.028818
C	0.033219	0.027441	2.865491
C	1.217563	0.025872	2.109353
C	1.177044	0.003922	0.712405
H	-0.056193	-0.027558	-1.056653
H	0.072423	0.039655	3.949767
H	2.175811	0.032703	2.620775
H	2.105732	0.000279	0.152493
H	-4.126850	1.228383	-0.750014
H	-2.360512	1.620594	-1.136747
C	-1.145818	-0.005248	2.148407
C	-1.216990	-0.010131	0.790828
C	-3.077153	0.988513	-0.626464
C	-2.661601	-0.010566	0.310709
H	-3.255253	0.069608	1.277043
H	-2.922417	-1.038251	0.006774



**C<sub>8</sub>H<sub>8</sub><sup>#</sup> 'biradical #1'**

B3LYP/6-311+G(d,p)

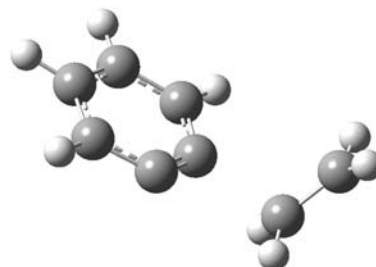
Zero-point correction

ZP = 0.126474

Electronic energy (including ZP)

E = -309.446193

C	0.309795	0.244988	0.034933
C	-0.584544	1.058674	0.480493
C	0.137578	-1.125086	-0.105179
C	-1.111950	-1.592065	0.323444
C	-2.080234	-0.716188	0.835657
C	-1.834310	0.662253	0.936835
H	0.895350	-1.796797	-0.495590
H	-1.332328	-2.652375	0.258069
H	-3.042940	-1.109571	1.147661
H	-2.589243	1.338587	1.322641
C	2.381746	0.695787	-1.748857
C	2.208178	0.921065	-0.408402
H	2.110386	1.443593	-2.484785
H	2.694007	-0.271247	-2.126632
H	2.042778	1.930368	-0.056174
H	2.661411	0.251002	0.314369

**C<sub>8</sub>H<sub>8</sub><sup>#</sup> 'biradical #2'**

B3LYP/6-311+G(d,p)

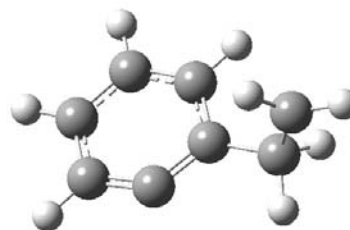
Zero-point correction

ZP = 0.127743

Electronic energy (including ZP)

E = -309.474517

C	-0.123192	0.542512	-0.201399
C	-1.108699	-0.385318	-0.455064
C	0.745053	0.212081	0.855969
C	0.586786	-0.972877	1.572885
C	-0.438478	-1.866473	1.258267
C	-1.319989	-1.569723	0.209877
H	1.548190	0.897649	1.111074
H	1.267570	-1.200796	2.385315
H	-0.557182	-2.786611	1.820496
H	-2.125295	-2.246430	-0.053954
C	1.164294	1.752165	-1.996102
C	0.048730	1.817432	-1.004554
H	1.467326	0.805312	-2.424870
H	1.588032	2.662419	-2.403493
H	-0.901397	2.036418	-1.516459
H	0.209296	2.660957	-0.321131

**C<sub>8</sub>H<sub>8</sub><sup>#</sup> 'biradical ↔ edge-on #'**

B3LYP/6-311+G(d,p)

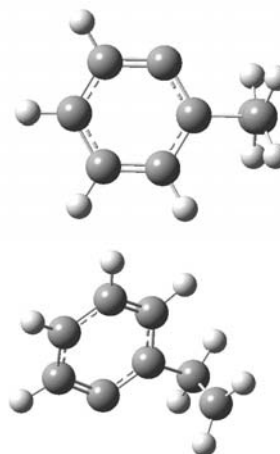
Zero-point correction

ZP = 0.128344

Electronic energy (including ZP)

E = -309.451220

C	0.627859	0.034928	0.165294
C	-0.061136	1.254520	0.156370
C	-0.100685	-1.193970	0.174531
C	-1.479360	-1.153142	0.125930
C	-2.156918	0.079991	0.149867
C	-1.440895	1.276431	0.283653
H	0.420663	-2.141253	0.286596
H	-2.047596	-2.076740	0.114204
H	-3.239491	0.098953	0.067337
H	-1.978544	2.213227	0.401932
C	2.163875	0.006374	0.284007
C	2.066198	0.013943	-1.165836
H	1.989806	0.948069	-1.702969
H	2.018510	-0.908890	-1.726854
H	2.533546	-0.907011	0.743406
H	2.565304	0.898740	0.751086



## Intermediates ( $o\text{-C}_6\text{H}_4 + \text{C}_3\text{H}_6$ )

### $\text{C}_9\text{H}_{10}$ 'edge-on (cis)'

B3LYP/6-311+G(d,p)

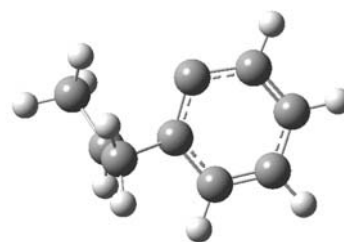
Zero-point correction

ZP = 0.158674

Electronic energy (including ZP)

E = -348.761214

C	0.680336	-1.261513	-0.181975
C	1.559478	1.365358	0.250485
C	2.426521	0.380030	-0.188096
C	1.991225	-0.955564	-0.405714
H	0.319865	-2.279969	-0.309031
H	1.969104	2.359424	0.420555
H	3.472052	0.618056	-0.372907
H	2.695360	-1.712554	-0.730817
H	-1.397637	-1.705985	1.457019
H	-1.754602	0.055906	1.836620
C	0.167811	1.153798	0.456659
C	-0.221416	-0.209843	0.230535
C	-1.485700	-0.687945	1.099158
C	-1.771614	-0.427162	-0.286622
H	-1.803051	-1.291492	-0.941770
C	-2.552272	0.770412	-0.760089
H	-2.283459	1.034523	-1.785471
H	-3.620452	0.525304	-0.738988
H	-2.363408	1.631352	-0.121259



### $\text{C}_9\text{H}_{10}$ 'edge-on (trans)'

B3LYP/6-311+G(d,p)

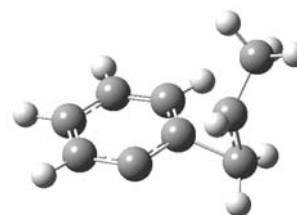
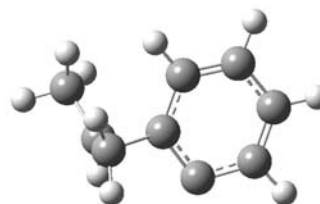
Zero-point correction

ZP = 0.158876

Electronic energy (including ZP)

E = -348.760641

C	0.266839	1.045537	0.478222
C	1.968964	-1.007129	-0.403468
C	2.429351	0.285969	-0.235680
C	1.577182	1.328123	0.221854
H	-0.394659	1.821369	0.852358
C	-0.209703	-0.300652	0.258652
C	0.616381	-1.394318	-0.185572
H	1.972103	2.326037	0.372936
H	3.469179	0.526009	-0.447892
H	2.682171	-1.761465	-0.730163
C	-1.747907	-0.460918	-0.311183
C	-1.507887	-0.737082	1.080843
H	-1.740752	-1.320929	-0.969320
H	-1.436708	-1.760998	1.419130
H	-1.812332	-0.005307	1.820233
C	-2.495910	0.746852	-0.814535
H	-2.089770	1.101679	-1.764478
H	-3.539528	0.461182	-0.984574
H	-2.493560	1.574128	-0.103031



**C<sub>9</sub>H<sub>10</sub> 'biradical'**

B3LYP/6-311+G(d,p)

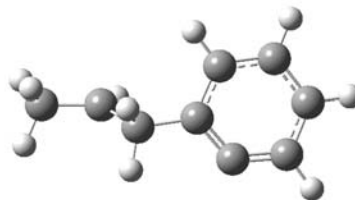
Zero-point correction

ZP = 0.156222

Electronic energy (including ZP)

E = -348.772941

C	0.085880	-0.213736	0.304861
C	0.970192	-1.239782	0.056066
C	0.648279	1.076512	0.268310
C	2.002540	1.262630	-0.004239
C	2.838782	0.172013	-0.249946
C	2.312321	-1.126292	-0.220152
H	0.009686	1.934799	0.456258
H	2.410523	2.267000	-0.023322
H	3.892022	0.323752	-0.461094
H	2.940711	-1.990506	-0.405451
C	-1.384892	-0.437790	0.587789
H	-1.555424	-1.519451	0.715737
H	-1.638806	0.005139	1.562943
C	-2.300702	0.110816	-0.461459
H	-1.900750	0.290228	-1.453466
C	-3.775927	0.120354	-0.251503
H	-4.289234	0.724184	-1.003709
H	-4.205952	-0.894139	-0.305224
H	-4.041621	0.510646	0.738975

**Transition States (o-C<sub>6</sub>H<sub>4</sub> + C<sub>3</sub>H<sub>6</sub>)****C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'edge-on #1, trans'**

B3LYP/6-311+G(d,p)

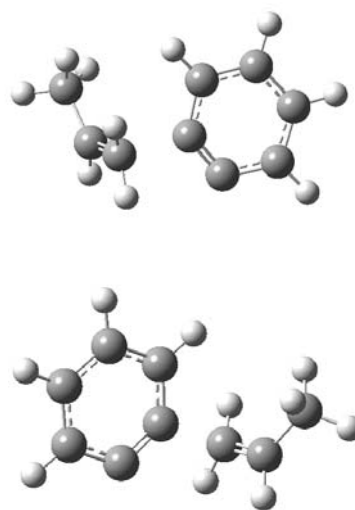
Zero-point correction

ZP = 0.155760

Electronic energy (including ZP)

E = -348.746395

C	0.389601	0.989997	0.450603
C	2.237662	-0.985710	-0.389054
C	2.628713	0.350681	-0.248524
C	1.715126	1.328727	0.173187
H	-0.311035	1.729634	0.824883
C	0.089391	-0.360988	0.279762
C	0.891497	-1.293693	-0.161907
H	2.041973	2.354973	0.302681
H	3.649353	0.642161	-0.480820
H	2.962870	-1.728719	-0.709569
C	-2.324390	-0.522877	-0.283300
C	-1.622417	-0.816435	0.872952
H	-2.346109	-1.278100	-1.064587
H	-1.452736	-1.853219	1.124673
H	-1.736442	-0.160277	1.731225
C	-2.926112	0.794569	-0.617334
H	-2.412742	1.258926	-1.469314
H	-3.969244	0.660797	-0.929952
H	-2.905514	1.488836	0.224745



**C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'edge-on #2, trans'**

B3LYP/6-311+G(d,p)

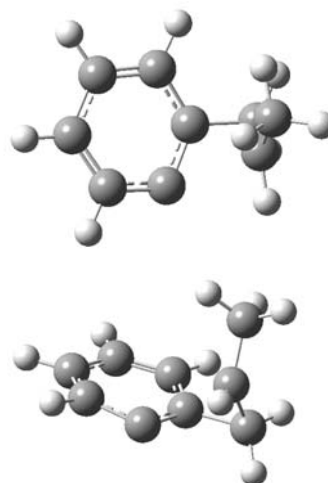
Zero-point correction

ZP = 0.157980

Electronic energy (including ZP)

E = -348.751545

C	-0.482960	1.271685	-0.338266
C	-1.540665	-1.279568	0.159509
C	-2.304439	-0.150686	0.364375
C	-1.762299	1.143836	0.128624
H	-0.026437	2.250816	-0.452951
C	0.225315	0.079841	-0.714264
C	-0.279891	-1.238180	-0.514731
H	-2.359528	2.022923	0.345800
H	-3.325293	-0.230221	0.729851
H	-1.955163	-2.245422	0.440595
C	1.731998	-0.515651	0.141782
C	1.667695	0.141087	-1.179808
H	1.882729	-1.582903	0.153209
H	1.903834	-0.489181	-2.031358
H	2.080492	1.145644	-1.238412
C	2.000251	0.213324	1.422368
H	1.401836	-0.187755	2.243514
H	3.054941	0.061504	1.685892
H	1.813336	1.285630	1.348292

**C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'ene #'**

B3LYP/6-311+G(d,p)

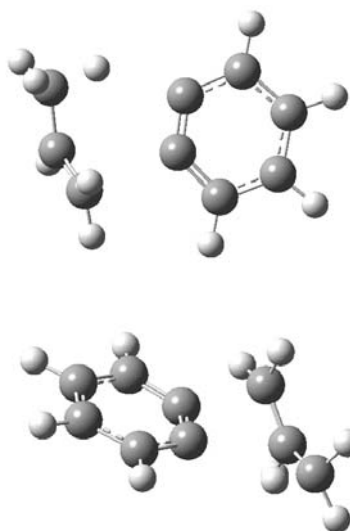
Zero-point correction

ZP = 0.155357

Electronic energy (including ZP)

E = -348.756465

C	1.073303	-1.352714	-0.049854
C	1.581116	1.468919	0.075792
C	2.625992	0.541506	-0.061985
C	2.379258	-0.838526	-0.122432
H	0.873347	-2.416931	-0.086347
H	1.786323	2.533291	0.123233
H	3.649564	0.897805	-0.127204
H	3.211312	-1.527359	-0.226349
H	-1.794875	-2.226078	0.057190
H	-1.843288	-1.021552	1.450294
C	0.301463	0.913510	0.131274
C	0.133119	-0.349725	0.082645
C	-1.961400	-1.207785	0.388937
C	-2.579584	-0.306011	-0.414208
H	-2.764088	-0.578899	-1.450405
C	-2.736174	1.103037	-0.035594
H	-3.377836	1.675946	-0.705158
H	-3.050232	1.242076	1.001081
H	-1.686152	1.530289	-0.081484





**C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'H-transfer #, cis'**

B3LYP/6-311+G(d,p)

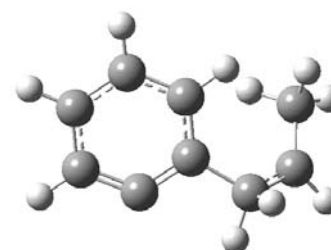
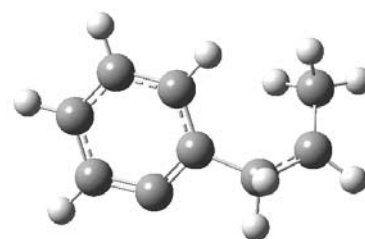
Zero-point correction

ZP = 0.154968

Electronic energy (including ZP)

E = -348.736717

C	-0.373730	0.936736	0.569178
C	-2.166679	-0.966228	-0.484975
C	-2.579607	0.355111	-0.257247
C	-1.689932	1.293890	0.273255
H	0.308426	1.678003	0.980049
H	-2.872402	-1.694960	-0.872965
H	-3.604290	0.644501	-0.473783
H	-2.026895	2.307883	0.459104
H	3.457906	-1.021925	-0.153181
C	-0.859480	-1.292156	-0.162740
C	0.032554	-0.383155	0.319947
C	2.583872	-0.384603	-0.052008
C	1.422128	-0.972572	0.575525
H	1.334755	-2.048896	0.273190
H	1.552051	-1.058413	1.668048
C	2.630572	0.951346	-0.675959
H	1.777128	1.086176	-1.357090
H	2.515670	1.757080	0.067777
H	3.559460	1.120336	-1.220996

**C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'H-transfer #, trans'**

B3LYP/6-311+G(d,p)

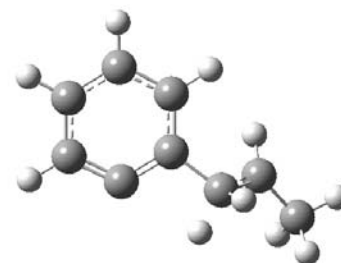
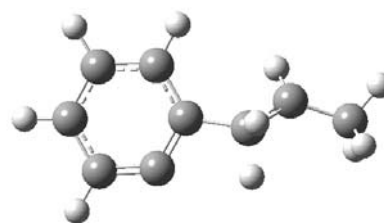
Zero-point correction

ZP = 0.154499

Electronic energy (including ZP)

E = -348.737992

C	-0.787727	1.198317	0.221537
C	-2.123006	-1.263087	-0.187084
C	-2.813811	-0.044103	-0.280029
C	-2.153096	1.169952	-0.074737
H	-0.290321	2.149168	0.388807
H	-2.651192	-2.199784	-0.337335
H	-3.876353	-0.046662	-0.506482
H	-2.708096	2.099377	-0.141357
H	2.017772	1.132470	-0.946571
C	-0.770877	-1.204534	0.104317
C	-0.107758	-0.023562	0.297171
C	2.344380	0.374585	-0.239768
C	1.361343	-0.263315	0.590715
H	1.440322	-1.396996	0.488821
H	1.557165	-0.139014	1.667922
C	3.743079	-0.096583	-0.338992
H	3.866039	-0.752085	-1.218823
H	4.435972	0.737734	-0.491488
H	4.053537	-0.670234	0.537716



**C<sub>9</sub>H<sub>10</sub><sup>#</sup> (biradical #1, trans)**

B3LYP/6-311+G(d,p)

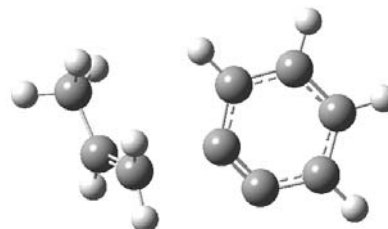
Zero-point correction

ZP = 0.154736

Electronic energy (including ZP)

E = -348.745219

C	0.176337	-0.371298	0.246001
C	1.026870	-1.266621	-0.127694
C	0.444764	0.981163	0.410797
C	1.777121	1.333295	0.157175
C	2.721416	0.371254	-0.228582
C	2.366397	-0.978809	-0.368238
H	-0.282731	1.719252	0.731140
H	2.082230	2.368490	0.269350
H	3.743847	0.678683	-0.427048
H	3.103502	-1.718692	-0.662799
C	-1.738097	-0.900127	0.769414
H	-1.511699	-1.946621	0.918160
H	-1.740214	-0.295413	1.671493
C	-2.516985	-0.526903	-0.296835
H	-2.649820	-1.238028	-1.108688
C	-3.090823	0.833965	-0.505861
H	-2.607403	1.340481	-1.351576
H	-4.156286	0.770629	-0.755843
H	-2.983442	1.465712	0.378742

**C<sub>9</sub>H<sub>10</sub><sup>#</sup> 'biradical ↔ edge-on'**

B3LYP/6-311+G(d,p)

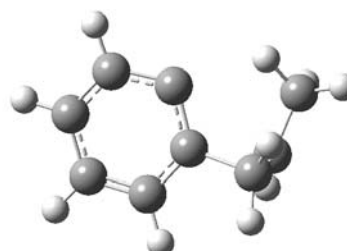
Zero-point correction

ZP = 0.157323

Electronic energy (including ZP)

E = -348.758458

C	0.146646	-0.293252	0.355094
C	-0.186822	1.051679	0.505695
C	-0.755518	-1.282647	-0.122907
C	-2.039849	-0.892382	-0.442788
C	-2.429511	0.443673	-0.228906
C	-1.542095	1.366582	0.326187
H	-0.472406	-2.332030	-0.165630
H	-2.754762	-1.614778	-0.820209
H	-3.430719	0.754818	-0.516006
H	-1.900326	2.373760	0.527970
C	1.540585	-0.822111	0.904845
C	1.958763	-0.429359	-0.406441
H	1.832856	-1.135667	-1.217735
H	1.483391	-1.882359	1.130366
H	1.896742	-0.223045	1.735406
C	2.534636	0.904516	-0.659586
H	3.483925	1.029550	-0.126768
H	2.677629	1.112212	-1.720027
H	1.822666	1.637355	-0.214526



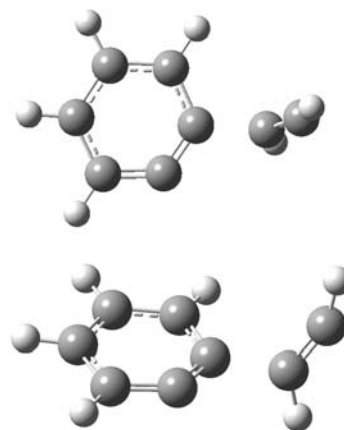
## Intermediates ( $o\text{-C}_6\text{H}_4 + \text{C}_2\text{H}_2$ )

**C<sub>8</sub>H<sub>6</sub> 'addition complex'** B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.103794

Electronic energy (including ZP) E = -308.209283

C	0	-0.031001	1.154764	-0.121477
C	0	-1.576776	-1.219756	0.075924
C	0	-2.184874	0.045115	0.111210
C	0	-1.418385	1.213486	0.013006
H	0	0.567297	2.051853	-0.244666
H	0	-2.170901	-2.122653	0.170624
H	0	-3.260272	0.117109	0.246791
H	0	-1.909974	2.179947	0.033576
H	0	3.146754	0.263889	1.522530
C	0	-0.196354	-1.206205	-0.004150
C	0	0.538171	-0.128095	-0.153608
C	0	2.931054	0.036272	0.498661
C	0	2.151377	-0.226338	-0.459952
H	0	2.347819	-0.505598	-1.486544

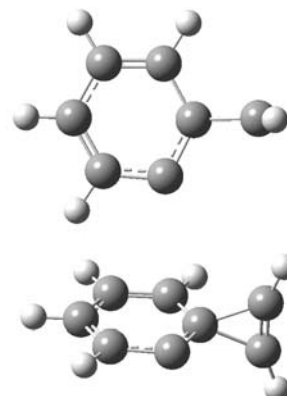


**C<sub>8</sub>H<sub>6</sub> 'edge-on'** B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.105034

Electronic energy (including ZP) E = -308.210814

C	-0.001031	1.208274	0.000148
C	-1.386070	-1.234179	-0.000180
C	-2.057437	-0.024273	-0.000043
C	-1.365937	1.218431	0.000123
H	0.568132	2.133444	0.000273
H	-1.986011	-2.142565	-0.000304
H	-3.145510	-0.006975	-0.000061
H	-1.919975	2.149978	0.000227
C	0.035280	-1.353638	-0.000167
C	0.684490	-0.069389	0.000004
C	2.162015	-0.039203	0.627638
C	2.162042	-0.039045	-0.627559
H	2.541662	-0.067669	-1.629400
H	2.541590	-0.068078	1.629489



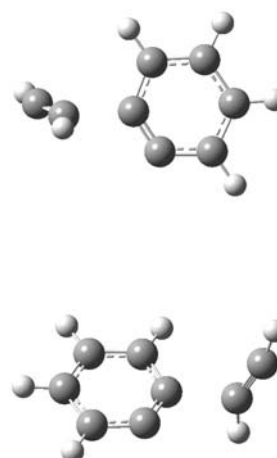
## Transition States ( $o\text{-C}_6\text{H}_4 + \text{C}_2\text{H}_2$ )

**C<sub>8</sub>H<sub>6</sub> # 'addition complex #'** B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.102802

Electronic energy (including ZP) E = -308.208661

C	0.038906	1.154094	0.118242
C	1.632781	-1.212176	-0.096690
C	2.216265	0.065120	-0.094363
C	1.433636	1.224257	0.011063
H	-0.577722	2.039614	0.221961
H	2.244274	-2.103050	-0.193016
H	3.293696	0.158602	-0.195473
H	1.914914	2.196466	0.012184
C	0.245847	-1.216164	-0.015012
C	-0.453530	-0.146997	0.117822
C	-3.005247	0.057902	-0.493084
C	-2.305321	-0.264812	0.471181
H	-2.329726	-0.592395	1.492348
H	-3.331686	0.345439	-1.466494



**C<sub>8</sub>H<sub>6</sub><sup>#</sup> 'edge-on #1'**

B3LYP/6-311+G(d,p)

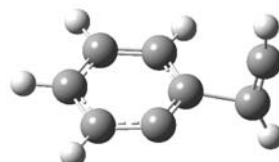
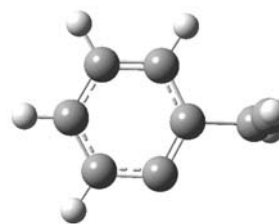
Zero-point correction

ZP = 0.103513

Electronic energy (including ZP)

E = -308.204034

C	-0.008896	1.187773	-0.110156
C	-1.445253	-1.229916	-0.002147
C	-2.098576	-0.001190	0.088142
C	-1.383605	1.212732	0.021682
H	0.561974	2.098346	-0.260901
H	-2.041559	-2.139487	0.011058
H	-3.176020	0.031323	0.229675
H	-1.913463	2.158202	0.046829
H	2.578260	0.123482	1.697751
C	-0.038760	-1.294806	0.019379
C	0.598890	-0.093586	-0.131346
C	2.478592	0.029494	0.640616
C	2.137655	-0.142281	-0.550867
H	2.503779	-0.288246	-1.552998

**C<sub>8</sub>H<sub>6</sub><sup>#</sup> 'edge-on #2'**

B3LYP/6-311+G(d,p)

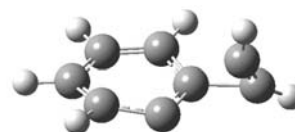
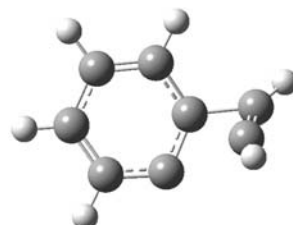
Zero-point correction

ZP = 0.104652

Electronic energy (including ZP)

E = -308.203301

C	-0.089275	1.283351	0.068285
C	-1.242095	-1.280050	-0.027076
C	-2.030450	-0.149138	0.020676
C	-1.447881	1.150728	0.090399
H	0.387862	2.240589	0.254041
H	-1.715786	-2.254707	0.060593
H	-3.114095	-0.232608	0.051644
H	-2.087166	2.015963	0.227163
C	0.151963	-1.212148	-0.335849
C	0.692268	0.107565	-0.246575
C	1.998483	-0.445886	0.636558
C	2.213721	0.263269	-0.398788
H	2.883307	0.838607	-1.010214
H	2.161779	-0.874833	1.606261

**C<sub>8</sub>H<sub>6</sub> 'H-transfer #'**

B3LYP/6-311+G(d,p)

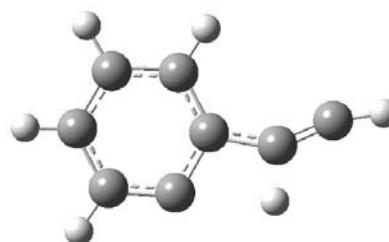
Zero-point correction

ZP = 0.101689

Electronic energy (including ZP)

E = -308.198734

C	0.542790	-0.047746	0.002250
C	-0.157922	-1.302487	-0.018204
C	-1.545695	-1.204954	-0.000005
C	-2.196356	0.034375	0.002402
C	-1.481836	1.233937	-0.002396
C	-0.093423	1.202015	0.000744
H	-2.158027	-2.103939	-0.003545
H	-3.281775	0.055377	0.005888
H	-2.008257	2.181504	-0.000485
H	0.477363	2.122488	0.015386
C	1.960285	-0.307973	0.022251
C	3.119294	0.203452	-0.020792
H	1.911999	-1.475891	0.068727
H	4.175881	0.356754	-0.003465



Remark: TS did not fully converge, but only 1 imaginary frequency. See text.

## PRODUCTS

### $o\text{-C}_6\text{H}_4 + \text{C}_2\text{H}_4$

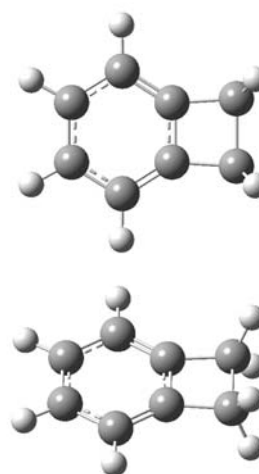
#### **$\text{C}_8\text{H}_8$ Benzocyclobutene**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.133856

Electronic energy (including ZP) E = -309.574708

C	0.452878	-0.696832	0.000000
C	0.452878	0.696832	0.000000
C	-0.718896	-1.436783	0.000000
C	-1.912755	-0.700160	0.000000
C	-1.912755	0.700160	0.000000
C	-0.718896	1.436783	0.000000
H	-0.734941	-2.521438	0.000000
H	-2.862332	-1.224507	0.000000
H	-2.862332	1.224507	0.000000
H	-0.734941	2.521438	0.000000
C	1.972599	0.791332	0.000000
C	1.972599	-0.791332	0.000000
H	2.417854	1.246490	0.888446
H	2.417854	1.246490	-0.888446
H	2.417854	-1.246490	0.888446
H	2.417854	-1.246490	-0.888446



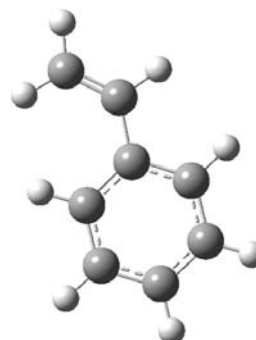
#### **$\text{C}_8\text{H}_8$ Styrene**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.132759

Electronic energy (including ZP) E = -309.598034

C	-0.000293	0.559108	0.002427
C	-1.006537	-0.421491	-0.013851
C	1.335703	0.130242	0.009022
C	1.660082	-1.224294	-0.002603
C	0.650057	-2.182744	-0.020008
C	-0.685229	-1.773229	-0.025180
H	2.127898	0.871924	0.022582
H	2.700551	-1.529536	0.002216
H	0.897061	-3.238277	-0.028615
H	-1.478007	-2.513084	-0.037163
C	-1.477277	2.602595	-0.019180
C	-0.282737	2.003697	0.013145
H	-2.410489	2.052171	-0.060062
H	-1.555904	3.682951	-0.006851
H	-2.049317	-0.126231	-0.015883
H	0.602392	2.635258	0.050004



$\sigma\text{-C}_6\text{H}_4 + \text{C}_3\text{H}_6$

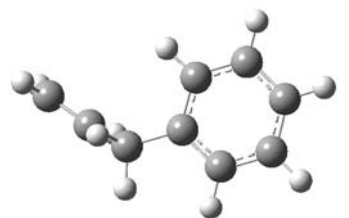
**C<sub>9</sub>H<sub>10</sub> Allylbenzene**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.160948

Electronic energy (including ZP) E = -348.890052

C	0.998687	-1.276172	-0.008505
C	0.003433	-0.328305	-0.261559
C	0.360683	1.025423	-0.274530
C	1.676971	1.418563	-0.047596
C	2.661996	0.462532	0.202371
C	2.318537	-0.886835	0.222169
H	0.740375	-2.330466	0.005219
H	-0.401109	1.775661	-0.459639
H	1.935023	2.471858	-0.064439
H	3.686822	0.768318	0.380447
H	3.075882	-1.638457	0.416250
C	-1.433813	-0.750402	-0.521513
H	-1.740101	-0.429868	-1.523481
H	-1.481286	-1.845483	-0.514990
C	-2.408539	-0.208663	0.492393
H	-2.198877	-0.463192	1.529769
C	-3.471777	0.539806	0.207119
H	-3.713320	0.820283	-0.814082
H	-4.140474	0.895663	0.982855



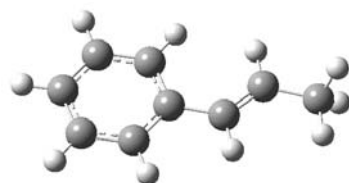
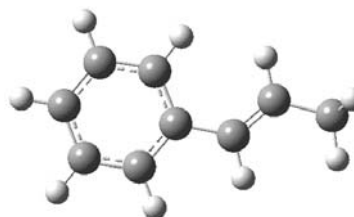
**C<sub>9</sub>H<sub>10</sub> E-Phenylpropene**

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.160665

Electronic energy (including ZP) E = -348.899545

C	-0.058378	-0.205421	-0.000166
C	-0.583845	1.098447	-0.000229
C	-1.956138	1.317081	-0.000060
C	-2.845310	0.240195	0.000156
C	-2.342964	-1.058583	0.000175
C	-0.967133	-1.275569	0.000004
H	0.084912	1.951296	-0.000465
H	-2.336613	2.332728	-0.000124
H	-3.915265	0.414407	0.000276
H	-3.021232	-1.904759	0.000317
H	-0.585002	-2.291468	0.000019
C	1.383332	-0.499558	-0.000312
H	1.628315	-1.560720	-0.000915
C	2.397763	0.373650	0.000291
H	2.189643	1.441427	0.001011
C	3.847725	-0.005861	0.000098
H	4.362424	0.401171	-0.877958
H	4.362378	0.400003	0.878721
H	3.980130	-1.090373	-0.000626



**C<sub>9</sub>H<sub>10</sub> Z-Phenylpropene**

B3LYP/6-311+G(d,p)

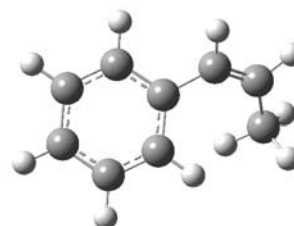
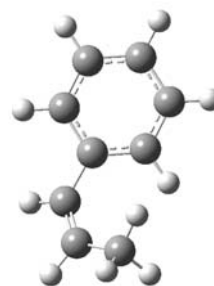
Zero-point correction

ZP = 0.161078

Electronic energy (including ZP)

E = -348.895067

C	0.054038	0.069832	0.074635
C	1.454281	0.173290	0.103696
C	2.082683	1.413433	0.017107
C	1.328881	2.579296	-0.105875
C	-0.062181	2.493095	-0.157017
C	-0.688360	1.253478	-0.076598
H	2.056996	-0.724161	0.162421
H	3.165766	1.467451	0.034823
H	1.820042	3.543388	-0.173832
H	-0.659069	3.392157	-0.264129
H	-1.771096	1.194724	-0.121469
C	-0.663742	-1.216652	0.152629
H	-1.582065	-1.252757	-0.429684
C	-0.358716	-2.311765	0.864694
H	-1.036218	-3.157017	0.765477
C	0.779171	-2.518376	1.822086
H	1.230253	-1.578989	2.144121
H	0.429167	-3.052922	2.710597
H	1.569068	-3.136956	1.378238

**C<sub>9</sub>H<sub>10</sub> 1-Methylbenzocyclobutene** B3LYP/6-311+G(d,p)

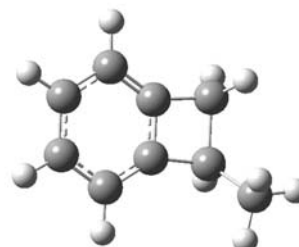
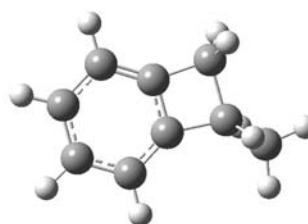
Zero-point correction

ZP = 0.161704

Electronic energy (including ZP)

E = -348.873631

C	-1.454742	1.294014	0.186350
C	-0.724152	-1.454199	-0.221769
C	-2.053176	-1.073261	0.015853
C	-2.409428	0.266520	0.213379
H	-1.746183	2.327331	0.341742
C	-0.145198	0.902956	-0.043963
C	0.208574	-0.428844	-0.245685
H	-3.450908	0.511228	0.392538
H	-2.827976	-1.831818	0.046649
H	-0.465214	-2.496323	-0.376528
C	1.690683	-0.109492	-0.435018
C	1.283192	1.405311	-0.191541
H	2.032106	-0.277495	-1.462124
H	1.470363	2.076432	-1.034310
H	1.720952	1.842541	0.710647
C	2.681017	-0.721687	0.550854
H	2.766238	-1.802367	0.402677
H	3.677815	-0.287677	0.424664
H	2.362189	-0.549754	1.583294



## $\text{o-C}_6\text{H}_4 + \text{C}_2\text{H}_2$

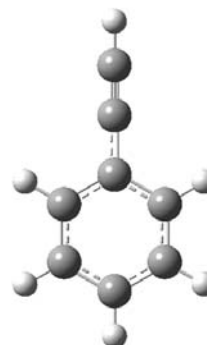
### $\text{C}_8\text{H}_6$ Phenylacetylene

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.109174

Electronic energy (including ZP) E = -308.368075

C	-0.000155	0.593899	0.000000
C	-1.210678	-0.119782	0.000000
C	-1.205871	-1.510456	0.000000
C	0.000848	-2.209777	0.000000
C	1.207064	-1.509602	0.000000
C	1.210862	-0.118923	0.000000
H	-2.146394	-2.049630	0.000000
H	0.001240	-3.293801	0.000000
H	2.147968	-2.048108	0.000000
H	2.146345	0.427329	0.000000
C	-0.000763	2.021952	0.000000
C	-0.001656	3.226993	0.000000
H	-2.146561	0.425785	0.000000
H	-0.002457	4.289346	0.000000



### $\text{C}_8\text{H}_6$ Benzocyclobutadiene

B3LYP/6-311+G(d,p)

Zero-point correction ZP = 0.109770

Electronic energy (including ZP) E = -308.328257

C	-0.000001	0.711200	0.522254
C	0.000001	-0.711200	0.522254
C	0.000002	-1.443153	-0.623477
C	0.000001	-0.688396	-1.844026
C	-0.000001	0.688396	-1.844026
C	-0.000002	1.443153	-0.623477
H	0.000003	-2.526936	-0.644274
H	0.000002	-1.220297	-2.788776
H	-0.000002	1.220297	-2.788776
H	-0.000003	2.526936	-0.644274
C	0.000001	0.675028	2.046570
C	-0.000001	-0.675028	2.046570
H	0.000000	1.425452	2.824942
H	0.000000	-1.425452	2.824942

