

## SUPPLEMENTARY MATERIAL

### Microwave Flash Pyrolysis: C<sub>9</sub>H<sub>8</sub> Interconversions and Dimerizations

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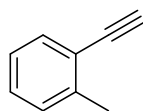
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#### I. Thermal rearrangements of o-ethynyltoluene computational data

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



**2**

Charge = 0 Multiplicity = 1

H				
C	1	B1		
C	2	B2	1	A1

C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
H	11	B11	4	A10	2	D9	0
C	11	B12	4	A11	2	D10	0
C	7	B13	3	A12	2	D11	0
H	14	B14	7	A13	3	D12	0
H	14	B15	7	A14	3	D13	0
H	14	B16	7	A15	3	D14	0

Variables:

B1	1.08343
B2	2.77555
B3	1.40492
B4	1.38942
B5	1.39337
B6	1.39622
B7	1.08388
B8	1.08424
B9	1.08497
B10	1.42822
B11	2.26806
B12	1.20559
B13	1.50659
B14	1.09401
B15	1.09403
B16	1.09131
A1	179.17257
A2	118.85916
A3	120.44657
A4	119.6117
A5	61.53646
A6	119.95071
A7	120.20811
A8	179.5936
A9	119.4786
A10	179.8879
A11	179.99085
A12	120.92173
A13	111.18897
A14	111.18581
A15	110.95377
D1	-0.03963
D2	180.
D3	-180.
D4	-0.03994
D5	0.

D6	180.
D7	179.78885
D8	0.
D9	2.06834
D10	41.565
D11	-179.995
D12	-120.72454
D13	120.5336
D14	-0.09165

E(RB+HF-LYP) = -347.805212570 A.U.

Zero-point correction=	0.136490 (Hartree/Particle)
Thermal correction to Energy=	0.195456
Thermal correction to Enthalpy=	0.198300
Thermal correction to Gibbs Free Energy=	-0.009151
Sum of electronic and zero-point Energies=	-347.668723
Sum of electronic and thermal Energies=	-347.609756
Sum of electronic and thermal Enthalpies=	-347.606912
Sum of electronic and thermal Free Energies=	-347.814364

### TS1

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	4	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
C	3	B9	2	A8	1	D7	0
C	7	B10	4	A9	2	D8	0
H	11	B11	7	A10	4	D9	0
H	11	B12	7	A11	4	D10	0
H	11	B13	7	A12	4	D11	0
H	4	B14	2	A13	1	D12	0
C	10	B15	3	A14	2	D13	0
H	16	B16	10	A15	3	D14	0

Variables:

B1	1.08417
B2	2.7957
B3	1.39431
B4	1.39467
B5	1.38808
B6	1.396
B7	1.08388
B8	1.08317
B9	1.63709

B10	1.50275
B11	1.09133
B12	1.09414
B13	1.09468
B14	1.08501
B15	1.25851
B16	1.07056
A1	179.4142
A2	119.79047
A3	120.16947
A4	119.54178
A5	121.68414
A6	120.45876
A7	120.68235
A8	166.65094
A9	121.02944
A10	110.96505
A11	111.70858
A12	110.19885
A13	119.4849
A14	74.1746
A15	172.92766
D1	-19.58026
D2	179.95718
D3	-179.74233
D4	-179.69243
D5	0.00802
D6	178.92362
D7	69.99526
D8	-178.99558
D9	7.0112
D10	-113.91617
D11	128.13359
D12	0.22088
D13	175.35009
D14	179.53748

E(RB+HF-LYP) = -347.714892580 A.U.

Imaginary Mode = -246.1795

Zero-point correction=	0.133763 (Hartree/Particle)
Thermal correction to Energy=	0.191185
Thermal correction to Enthalpy=	0.194029
Thermal correction to Gibbs Free Energy=	-0.008091
Sum of electronic and zero-point Energies=	-347.581130
Sum of electronic and thermal Energies=	-347.523707
Sum of electronic and thermal Enthalpies=	-347.520864
Sum of electronic and thermal Free Energies=	-347.722983

**TS2**

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
C	7	B12	3	A11	2	D10	0
H	13	B13	7	A12	3	D11	0
H	13	B14	7	A13	3	D12	0
H	13	B15	7	A14	3	D13	0
H	12	B16	11	A15	4	D14	0

Variables:

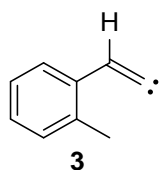
B1	1.08405
B2	2.77692
B3	1.40214
B4	1.38944
B5	1.39295
B6	1.39577
B7	1.08356
B8	1.08388
B9	1.08476
B10	1.43867
B11	1.26343
B12	1.50604
B13	1.09453
B14	1.09452
B15	1.09081
B16	1.27459
A1	179.62841
A2	119.65184
A3	120.06083
A4	119.70341
A5	61.65552
A6	119.81231
A7	120.18769
A8	179.63586
A9	120.97879
A10	173.69263
A11	121.39472
A12	111.23889
A13	111.23846
A14	110.96893
A15	60.79395

D1	-1.17068
D2	180.
D3	-179.98964
D4	-1.17507
D5	0.00578
D6	179.9967
D7	178.67617
D8	0.
D9	179.97167
D10	179.99474
D11	-120.45028
D12	120.61253
D13	0.07721
D14	179.75189

E(UB+HF-LYP) = -347.729745390 A.U.

Imaginary Mode = -325.4379

Zero-point correction=	0.130728 (Hartree/Particle)
Thermal correction to Energy=	0.189390
Thermal correction to Enthalpy=	0.192234
Thermal correction to Gibbs Free Energy=	-0.020084
Sum of electronic and zero-point Energies=	-347.599017
Sum of electronic and thermal Energies=	-347.540355
Sum of electronic and thermal Enthalpies=	-347.537512
Sum of electronic and thermal Free Energies=	-347.749829



Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0

C	7	B12	3	A11	2	D10	0
H	13	B13	7	A12	3	D11	0
H	13	B14	7	A13	3	D12	0
H	13	B15	7	A14	3	D13	0
H	11	B16	4	A15	2	D14	0

Variables:

B1	1.0845
B2	2.77665
B3	1.40101
B4	1.39016
B5	1.39324
B6	1.39606
B7	1.08379
B8	1.08403
B9	1.08482
B10	1.46203
B11	1.30218
B12	1.50187
B13	1.09691
B14	1.09691
B15	1.09112
B16	1.1077
A1	179.6693
A2	119.44908
A3	119.98408
A4	119.64603
A5	61.3596
A6	119.95087
A7	120.1925
A8	179.66803
A9	120.36512
A10	139.37863
A11	121.66226
A12	111.07405
A13	111.07515
A14	111.77598
A15	119.7412
D1	0.21324
D2	179.99733
D3	180.
D4	0.21144
D5	0.
D6	-180.
D7	-179.86274
D8	0.
D9	-179.89949
D10	179.99724
D11	-120.60887
D12	120.61704
D13	0.00363
D14	-0.09997

E(RB+HF-LYP) = -347.730760270 A.U.

Zero-point correction=	0.134152 (Hartree/Particle)
Thermal correction to Energy=	0.193537
Thermal correction to Enthalpy=	0.196380
Thermal correction to Gibbs Free Energy=	-0.012152
Sum of electronic and zero-point Energies=	-347.596608
Sum of electronic and thermal Energies=	-347.537224
Sum of electronic and thermal Enthalpies=	-347.534380
Sum of electronic and thermal Free Energies=	-347.742912

### TS3

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	7	B11	3	A10	2	D9	0
H	12	B12	7	A11	3	D10	0
H	12	B13	7	A12	3	D11	0
C	11	B14	4	A13	2	D12	0
H	15	B15	11	A14	4	D13	0
H	15	B16	11	A15	4	D14	0

Variables:

B1	1.08304
B2	2.80222
B3	1.41677
B4	1.37438
B5	1.37507
B6	1.42473
B7	1.08387
B8	1.08448
B9	1.08415
B10	1.39911
B11	1.41706
B12	1.08358
B13	1.08587
B14	1.2855
B15	1.07975
B16	1.22759
A1	178.46852
A2	118.12958



A3	120.91942
A4	59.39831
A5	62.32703
A6	120.26166
A7	119.5904
A8	178.51774
A9	124.43877
A10	121.1819
A11	119.99437
A12	117.9545
A13	128.12402
A14	135.67389
A15	107.11024
D1	-58.33786
D2	179.83834
D3	122.19355
D4	-60.33915
D5	0.67379
D6	179.64576
D7	173.19982
D8	11.38638
D9	173.20466
D10	134.04646
D11	-14.30958
D12	152.41586
D13	150.92046
D14	-8.74327

E(RB+HF-LYP) = -347.713675836 A.U.

Imaginary Mode = -978.9589

Zero-point correction=	0.132297 (Hartree/Particle)
Thermal correction to Energy=	0.188745
Thermal correction to Enthalpy=	0.191589
Thermal correction to Gibbs Free Energy=	-0.004465
Sum of electronic and zero-point Energies=	-347.581379
Sum of electronic and thermal Energies=	-347.524931
Sum of electronic and thermal Enthalpies=	-347.522087
Sum of electronic and thermal Free Energies=	-347.718141

#### TS4

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0

H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
C	7	B12	3	A11	2	D10	0
H	13	B13	7	A12	3	D11	0
H	12	B14	11	A13	4	D12	0
H	13	B15	7	A14	3	D13	0
H	11	B16	4	A15	2	D14	0

Variables:

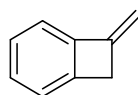
B1	1.08443
B2	2.80895
B3	1.39777
B4	1.39238
B5	1.39499
B6	1.39565
B7	1.08412
B8	1.08402
B9	1.08458
B10	1.46021
B11	1.33522
B12	1.47301
B13	1.09054
B14	1.1616
B15	1.09204
B16	1.08796
A1	179.03872
A2	120.1873
A3	120.49149
A4	59.52409
A5	60.05511
A6	119.82405
A7	119.70993
A8	179.18863
A9	127.12975
A10	123.15517
A11	125.96606
A12	114.90786
A13	126.92606
A14	116.95882
A15	119.76868
D1	81.58498
D2	-178.25096
D3	-96.7674
D4	83.95729
D5	-0.49225
D6	179.87478
D7	-157.4324
D8	-4.63673
D9	-174.82719

D10 177.00273  
 D11 -94.60922  
 D12 16.56605  
 D13 38.99493  
 D14 4.98764

E(RB+HF-LYP) = -347.714265434 A.U.

Imaginary Mode = -932.8380

Zero-point correction= 0.133054 (Hartree/Particle)  
 Thermal correction to Energy= 0.189363  
 Thermal correction to Enthalpy= 0.192207  
 Thermal correction to Gibbs Free Energy= -0.003840  
 Sum of electronic and zero-point Energies= -347.581211  
 Sum of electronic and thermal Energies= -347.524903  
 Sum of electronic and thermal Enthalpies= -347.522059  
 Sum of electronic and thermal Free Energies= -347.718105



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Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	7	B11	3	A10	2	D9	0
H	12	B12	7	A11	3	D10	0
H	12	B13	7	A12	3	D11	0
C	11	B14	4	A13	2	D12	0
H	15	B15	11	A14	4	D13	0
H	15	B16	11	A15	4	D14	0

Variables:

B1 1.08409  
 B2 2.87991  
 B3 1.39048  
 B4 1.39966  
 B5 1.40226  
 B6 1.38336  
 B7 1.08455

B8	1.08463
B9	1.08443
B10	1.4789
B11	1.52963
B12	1.09379
B13	1.09379
B14	1.33081
B15	1.08447
B16	1.08429
A1	179.1892
A2	123.13252
A3	120.93341
A4	121.79724
A5	57.85629
A6	119.39974
A7	118.82214
A8	178.93542
A9	145.33793
A10	144.45027
A11	115.7854
A12	115.7854
A13	136.78546
A14	121.44548
A15	121.31107
D1	180.
D2	180.
D3	180.
D4	180.
D5	0.
D6	180.
D7	0.
D8	0.
D9	180.
D10	-64.79902
D11	64.79902
D12	0.
D13	0.
D14	180.

E(RB+HF-LYP) = -347.803272353 A.U.

Zero-point correction=	0.138442 (Hartree/Particle)
Thermal correction to Energy=	0.194992
Thermal correction to Enthalpy=	0.197836
Thermal correction to Gibbs Free Energy=	0.000904
Sum of electronic and zero-point Energies=	-347.664830
Sum of electronic and thermal Energies=	-347.608280
Sum of electronic and thermal Enthalpies=	-347.605436
Sum of electronic and thermal Free Energies=	-347.802368

**TS5**

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	7	B11	3	A10	2	D9	0
H	12	B12	7	A11	3	D10	0
H	12	B13	7	A12	3	D11	0
C	11	B14	4	A13	2	D12	0
H	15	B15	11	A14	4	D13	0
H	15	B16	11	A15	4	D14	0

Variables:

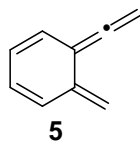
B1	1.08348
B2	2.8726
B3	1.41767
B4	1.37777
B5	1.37999
B6	1.41383
B7	1.0842
B8	1.08447
B9	1.08458
B10	1.38473
B11	1.4143
B12	1.0797
B13	1.08801
B14	1.3126
B15	1.09047
B16	1.08469
A1	178.55399
A2	121.44093
A3	121.66338
A4	58.15028
A5	59.52242
A6	119.7066
A7	119.53709
A8	178.54874
A9	133.80368
A10	132.81038
A11	118.35048
A12	122.57307
A13	151.97681
A14	120.91475
A15	122.34175

D1	82.05438
D2	-174.81875
D3	-91.39642
D4	92.75673
D5	-1.13174
D6	-179.94315
D7	-149.56555
D8	-13.19483
D9	170.90482
D10	-128.07452
D11	30.59277
D12	-43.9822
D13	-3.33022
D14	178.04061

E(RB+HF-LYP) = -347.729606731 A.U.

Imaginary Mode = -597.6125

Zero-point correction=	0.134541 (Hartree/Particle)
Thermal correction to Energy=	0.191124
Thermal correction to Enthalpy=	0.193968
Thermal correction to Gibbs Free Energy=	-0.004489
Sum of electronic and zero-point Energies=	-347.595066
Sum of electronic and thermal Energies=	-347.538483
Sum of electronic and thermal Enthalpies=	-347.535639
Sum of electronic and thermal Free Energies=	-347.734096



Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
H	12	B12	11	A11	4	D10	0
H	12	B13	11	A12	4	D11	0
C	7	B14	3	A13	2	D12	0
H	15	B15	7	A14	3	D13	0

H 15 B16 7 A15 3 D14 0

Variables:

B1	1.08332
B2	2.83406
B3	1.46546
B4	1.34812
B5	1.34921
B6	1.45945
B7	1.08405
B8	1.08426
B9	1.08482
B10	1.32435
B11	1.29927
B12	1.08853
B13	1.08854
B14	1.35022
B15	1.08287
B16	1.08331
A1	179.61175
A2	117.39543
A3	121.17692
A4	59.06828
A5	63.47863
A6	120.10686
A7	120.13629
A8	179.51654
A9	119.29631
A10	179.80363
A11	121.69677
A12	121.68525
A13	120.45302
A14	122.13746
A15	120.50873
D1	-1.38977
D2	-179.99171
D3	178.63154
D4	-1.36761
D5	0.
D6	-179.9957
D7	178.12343
D8	0.03606
D9	19.18843
D10	-109.24364
D11	70.82232
D12	179.97276
D13	180.
D14	0.

$E(\text{RB}+\text{HF}-\text{LYP}) = -347.766610202 \text{ A.U.}$

Zero-point correction= 0.135513 (Hartree/Particle)

Thermal correction to Energy= 0.194571  
 Thermal correction to Enthalpy= 0.197415  
 Thermal correction to Gibbs Free Energy= -0.010724  
 Sum of electronic and zero-point Energies= -347.631097  
 Sum of electronic and thermal Energies= -347.572039  
 Sum of electronic and thermal Enthalpies= -347.569195  
 Sum of electronic and thermal Free Energies= -347.777334

## TS6

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
H	12	B12	11	A11	4	D10	0
H	12	B13	11	A12	4	D11	0
C	7	B14	3	A13	2	D12	0
H	15	B15	7	A14	3	D13	0
H	15	B16	7	A15	3	D14	0

Variables:

B1	1.08328
B2	2.83459
B3	1.42484
B4	1.37176
B5	1.37741
B6	1.41689
B7	1.08398
B8	1.08485
B9	1.08447
B10	1.394
B11	1.37483
B12	1.08742
B13	1.09348
B14	1.41589
B15	1.082
B16	1.08715
A1	178.69922
A2	118.58584
A3	121.60019
A4	58.61839
A5	61.32902

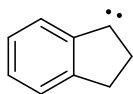


A6	120.40255
A7	119.40048
A8	178.03344
A9	125.70097
A10	115.41333
A11	122.94622
A12	117.58186
A13	125.46144
A14	119.45286
A15	119.2404
D1	-32.67314
D2	177.04093
D3	144.45968
D4	-37.35874
D5	0.53759
D6	178.90424
D7	-163.4676
D8	9.61304
D9	154.36832
D10	145.73959
D11	-61.63278
D12	-179.9241
D13	125.88159
D14	-22.57083

E(RB+HF-LYP) = -347.711323294 A.U.

Imaginary Mode = -540.8735

Zero-point correction=	0.134861 (Hartree/Particle)
Thermal correction to Energy=	0.190784
Thermal correction to Enthalpy=	0.193627
Thermal correction to Gibbs Free Energy=	-0.001175
Sum of electronic and zero-point Energies=	-347.576462
Sum of electronic and thermal Energies=	-347.520540
Sum of electronic and thermal Enthalpies=	-347.517696
Sum of electronic and thermal Free Energies=	-347.712498



23

Charge = 0 Multiplicity = 1

H				
C	1	B1		
C	2	B2	1	A1

C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
H	12	B12	11	A11	4	D10	0
H	12	B13	11	A12	4	D11	0
C	7	B14	3	A13	2	D12	0
H	15	B15	7	A14	3	D13	0
H	15	B16	7	A15	3	D14	0

Variables:

B1	1.08397
B2	2.83124
B3	1.40957
B4	1.3859
B5	1.39551
B6	1.392
B7	1.08391
B8	1.08523
B9	1.08488
B10	1.44314
B11	1.49942
B12	1.09849
B13	1.09852
B14	1.50201
B15	1.09539
B16	1.09539
A1	178.49504
A2	119.0208
A3	121.73395
A4	58.50816
A5	59.99028
A6	120.56609
A7	119.17204
A8	178.5278
A9	125.98429
A10	103.741
A11	108.09128
A12	108.06125
A13	129.91268
A14	111.46756
A15	111.4714
D1	0.00581
D2	180.
D3	-179.99544
D4	0.00534
D5	0.

D6	180.
D7	-179.96312
D8	-0.00403
D9	179.98643
D10	124.25962
D11	-124.16995
D12	-179.99731
D13	59.44658
D14	-59.40938

E(RB+HF-LYP) = -347.752114920 A.U.

Zero-point correction=	0.137665 (Hartree/Particle)
Thermal correction to Energy=	0.194079
Thermal correction to Enthalpy=	0.196923
Thermal correction to Gibbs Free Energy=	-0.000901
Sum of electronic and zero-point Energies=	-347.614450
Sum of electronic and thermal Energies=	-347.558036
Sum of electronic and thermal Enthalpies=	-347.555192
Sum of electronic and thermal Free Energies=	-347.753016

## TS7

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	11	B11	4	A10	2	D9	0
H	12	B12	11	A11	4	D10	0
C	7	B13	3	A12	2	D11	0
H	14	B14	7	A13	3	D12	0
H	14	B15	7	A14	3	D13	0
H	12	B16	11	A15	4	D14	0

Variables:

B1	1.08402
B2	2.82533
B3	1.39582
B4	1.3939
B5	1.39759
B6	1.38981
B7	1.08425

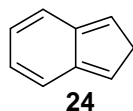
B8	1.08467
B9	1.08511
B10	1.48684
B11	1.41379
B12	1.08738
B13	1.50737
B14	1.09533
B15	1.09707
B16	1.27372
A1	179.26009
A2	119.73749
A3	121.24421
A4	59.03984
A5	59.43819
A6	120.04957
A7	119.47451
A8	179.15055
A9	127.14027
A10	102.68204
A11	122.8384
A12	130.35875
A13	113.38266
A14	112.81983
A15	59.85298
D1	-9.28422
D2	179.77184
D3	170.58767
D4	-9.12022
D5	0.11223
D6	-179.95697
D7	177.56532
D8	2.97249
D9	-177.62342
D10	-174.12602
D11	-179.22959
D12	57.2715
D13	-63.9932
D14	104.78126

E(RB+HF-LYP) = -347.734019203 A.U.

Imaginary Mode = -1057.1968

Zero-point correction=	0.134740 (Hartree/Particle)
Thermal correction to Energy=	0.189327
Thermal correction to Enthalpy=	0.192170
Thermal correction to Gibbs Free Energy=	0.001353
Sum of electronic and zero-point Energies=	-347.599280

Sum of electronic and thermal Energies= -347.544693  
 Sum of electronic and thermal Enthalpies= -347.541849  
 Sum of electronic and thermal Free Energies= -347.732666



Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	3	B4	2	A3	1	D2	0
C	2	B5	1	A4	3	D3	0
C	2	B6	1	A5	6	D4	0
H	5	B7	3	A6	2	D5	0
H	7	B8	2	A7	1	D6	0
H	3	B9	2	A8	1	D7	0
C	6	B10	2	A9	1	D8	0
C	4	B11	3	A10	2	D9	0
H	12	B12	4	A11	3	D10	0
C	12	B13	4	A12	3	D11	0
H	11	B14	6	A13	2	D12	0
H	14	B15	12	A14	4	D13	0
H	14	B16	12	A15	4	D14	0

Variables:

B1	1.08467
B2	2.45386
B3	2.41424
B4	1.35745
B5	1.4415
B6	1.35745
B7	1.08467
B8	1.08455
B9	1.08455
B10	1.3611
B11	1.3611
B12	1.08142
B13	1.4996
B14	1.08142
B15	1.09994
B16	1.09994
A1	151.18665
A2	62.31922
A3	93.73965
A4	119.79873
A5	121.02267

A6	121.02267
A7	120.00161
A8	146.25874
A9	131.90352
A10	161.30448
A11	126.979
A12	108.7118
A13	126.979
A14	111.77951
A15	111.77951
D1	180.
D2	180.
D3	180.
D4	180.
D5	180.
D6	0.
D7	0.
D8	0.
D9	180.
D10	0.
D11	180.
D12	0.
D13	-121.03589
D14	121.03589

E(RB+HF-LYP) = -347.815945374 A.U.

Zero-point correction=	0.138476 (Hartree/Particle)
Thermal correction to Energy=	0.194678
Thermal correction to Enthalpy=	0.197522
Thermal correction to Gibbs Free Energy=	0.005340
Sum of electronic and zero-point Energies=	-347.677469
Sum of electronic and thermal Energies=	-347.621267
Sum of electronic and thermal Enthalpies=	-347.618424
Sum of electronic and thermal Free Energies=	-347.810606

## TS8

Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	3	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	3	A7	2	D6	0

H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
H	11	B11	4	A10	2	D9	0
C	11	B12	4	A11	2	D10	0
H	13	B13	11	A12	4	D11	0
C	7	B14	3	A13	2	D12	0
H	15	B15	7	A14	3	D13	0
H	13	B16	11	A15	4	D14	0

Variables:

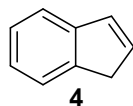
B1	1.08493
B2	2.8501
B3	1.41745
B4	1.37334
B5	1.37256
B6	1.4224
B7	1.08424
B8	1.08469
B9	1.08475
B10	1.40953
B11	1.07987
B12	1.48857
B13	1.08171
B14	1.40548
B15	1.07992
B16	1.24838
A1	179.54678
A2	120.30968
A3	120.76266
A4	58.63223
A5	60.56193
A6	119.96
A7	119.71957
A8	179.19832
A9	131.46383
A10	128.92498
A11	106.46425
A12	123.61176
A13	131.64196
A14	126.71788
A15	61.04619
D1	148.61147
D2	179.24856
D3	-32.10068
D4	148.96079
D5	-0.2231
D6	179.67415
D7	0.84371
D8	-0.56474
D9	5.99544
D10	-177.79972
D11	-168.24915

D12        -178.08629  
 D13        -0.05867  
 D14        99.56476

E(RB+HF-LYP) = -347.786691325 A.U.

Imaginary Mode = -1206.1506

Zero-point correction=                    0.135607 (Hartree/Particle)  
 Thermal correction to Energy=            0.190067  
 Thermal correction to Enthalpy=         0.192910  
 Thermal correction to Gibbs Free Energy= 0.003239  
 Sum of electronic and zero-point Energies= -347.651084  
 Sum of electronic and thermal Energies= -347.596625  
 Sum of electronic and thermal Enthalpies= -347.593781  
 Sum of electronic and thermal Free Energies= -347.783452



Charge = 0 Multiplicity = 1

H							
C	1	B1					
C	2	B2	1	A1			
C	2	B3	1	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	5	B5	2	A4	1	D3	0
C	3	B6	2	A5	1	D4	0
H	5	B7	2	A6	1	D5	0
H	6	B8	5	A7	2	D6	0
H	3	B9	2	A8	1	D7	0
C	4	B10	2	A9	1	D8	0
C	7	B11	3	A10	2	D9	0
H	12	B12	7	A11	3	D10	0
H	12	B13	7	A12	3	D11	0
H	11	B14	4	A13	2	D12	0
C	11	B15	4	A14	2	D13	0
H	16	B16	11	A15	4	D14	0

Variables:

B1        1.08484  
 B2        2.82332  
 B3        1.39481  
 B4        1.39597  
 B5        1.39706  
 B6        1.38723



B7	1.08445
B8	1.08431
B9	1.0854
B10	1.46632
B11	1.51106
B12	1.09723
B13	1.09723
B14	1.08292
B15	1.3454
B16	1.08219
A1	179.80095
A2	120.85453
A3	120.45243
A4	120.74036
A5	59.58336
A6	119.70421
A7	119.65326
A8	179.43268
A9	131.35063
A10	130.71635
A11	112.1244
A12	112.1244
A13	124.32261
A14	109.70848
A15	126.00599
D1	180.
D2	180.
D3	180.
D4	180.
D5	0.
D6	180.
D7	0.
D8	0.
D9	180.
D10	-59.83279
D11	59.83279
D12	0.
D13	180.
D14	180.

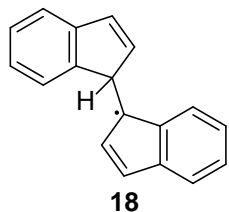
E(RB+HF-LYP) = -347.851053653 A.U.

Zero-point correction=	0.139886 (Hartree/Particle)
Thermal correction to Energy=	0.195271
Thermal correction to Enthalpy=	0.198115
Thermal correction to Gibbs Free Energy=	0.006114
Sum of electronic and zero-point Energies=	-347.711167
Sum of electronic and thermal Energies=	-347.655782

Sum of electronic and thermal Enthalpies= -347.652939  
Sum of electronic and thermal Free Energies= -347.844939

## II. Bi-indene to chrysene computational data

All UB3LYP/6-31G(d) theory.



Charge = 0 Multiplicity = 2

C,0,-1.5030870646,0.1639069598,0.1792461673  
C,0,-3.7143703834,-0.6686091616,-1.3201995631  
C,0,-2.7178290824,0.9183310897,0.1948715132  
C,0,-1.4091985581,-0.9937305751,-0.5884435965  
C,0,-2.5269396953,-1.4050381828,-1.3383360975  
C,0,-3.8185463903,0.5037593801,-0.5505953922  
H,0,-0.4928507871,-1.5744240699,-0.6160524683  
H,0,-2.4627039723,-2.3066625169,-1.9404383834  
H,0,-4.7444184578,1.0732148642,-0.5417851001  
H,0,-4.5649695187,-1.0034320576,-1.906711217  
C,0,-2.5074543568,2.0585744914,1.0680130063  
H,0,-3.2404820024,2.8254689726,1.2898313993  
C,0,-1.2001736487,1.993439569,1.5671592949  
H,0,-0.7480244918,2.7063137311,2.2470746434  
C,0,-0.5517887428,0.8543774405,1.0525919062  
C,0,0.8556647494,0.4349817166,1.3752838501  
C,0,0.9839508249,-0.9065139245,2.0891139185  
H,0,0.4243233653,-1.1408734454,2.9871736478  
C,0,1.8783431878,-1.7019003938,1.4683517105  
H,0,2.1732466084,-2.696095511,1.7874119621  
C,0,2.4064929312,-1.0229514121,0.2803544421  
C,0,3.0300670514,0.6956552499,-1.8220085853  
C,0,3.341908822,-1.4288474163,-0.6754531088  
C,0,1.791655873,0.2448133364,0.1861183959  
C,0,2.0950144306,1.1066058566,-0.8603775529  
C,0,3.6473107075,-0.5578796018,-1.7278458216  
H,0,3.8229744324,-2.4009280322,-0.6066739513  
H,0,1.6145856432,2.0781480313,-0.9405656014  
H,0,4.3697358891,-0.8578460962,-2.481644543  
H,0,3.275984278,1.3552932371,-2.6491210001  
H,0,1.2823986984,1.2089845007,2.0326946551

E(UB3LYP) = -693.740630776 A.U.

S\*\*2 = 0.7690

Zero-point correction=	0.248806 (Hartree/Particle)
Thermal correction to Energy=	0.261856
Thermal correction to Enthalpy=	0.262801
Thermal correction to Gibbs Free Energy=	0.207438
Sum of electronic and zero-point Energies=	-693.491824
Sum of electronic and thermal Energies=	-693.478774
Sum of electronic and thermal Enthalpies=	-693.477830
Sum of electronic and thermal Free Energies=	-693.533193

## TS9

Charge = 0 Multiplicity = 2

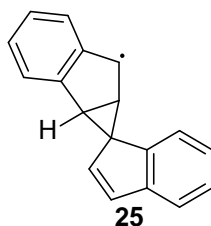
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C,0,0.41666544,1.2529040201,1.0384594674  
C,0,1.5872737481,0.8403270062,1.730828226  
C,0,2.5393041693,0.3357305163,0.7898558203  
C,0,1.9862924822,0.4255933783,-0.5222187372  
H,0,0.2571911214,1.6825065167,-1.1752460226  
H,0,-0.3391362107,1.9147603582,1.4397400367  
H,0,1.7192201681,0.8746861414,2.805938882  
C,0,-0.4637952244,0.0091712385,0.069348938  
C,0,-1.9050886188,0.2542275124,-0.0704528172  
C,0,-2.5717996141,-0.9786822253,0.1742046686  
C,0,-1.5530169094,-1.9847036997,0.4585011647  
C,0,-0.3215557455,-1.4095626306,0.3926366831  
H,0,-1.7586992969,-3.0252507597,0.6844259299  
H,0,0.6287100945,-1.9016350103,0.5550062146  
H,0,-2.1325049183,2.3482236588,-0.5818525631  
C,0,-2.6311242134,1.4008037449,-0.3872287795  
H,0,-4.6055063957,2.2069489936,-0.6980275098  
C,0,-4.0272859676,1.3202980578,-0.4522478696  
H,0,-5.7691883215,0.0664325605,-0.2627816719  
C,0,-4.6846342578,0.1092329336,-0.2066607288  
H,0,-4.4802570127,-1.9865363271,0.2894781511  
C,0,-3.9619770841,-1.0482072925,0.1065067329  
H,0,4.2628567598,-0.2792254877,1.9603801496  
C,0,3.8313552682,-0.1959822719,0.9662550857  
H,0,5.5548440029,-0.9986143837,-0.0327778973  
C,0,4.5515424968,-0.5987971931,-0.1547498102  
H,0,4.5867587564,-0.8137293104,-2.3023828824  
C,0,4.0033444222,-0.49557484,-1.4429154051  
H,0,2.2860281173,0.0771384316,-2.6293081919  
C,0,2.7100229808,0.0106577064,-1.6304254908

E(UB+HF-LYP) = -693.668494486 A.U.

S\*\*2 = 0.7787

Imaginary Mode = -458.8264

Zero-point correction=	0.248507 (Hartree/Particle)
Thermal correction to Energy=	0.260922
Thermal correction to Enthalpy=	0.261866
Thermal correction to Gibbs Free Energy=	0.208796
Sum of electronic and zero-point Energies=	-693.419988
Sum of electronic and thermal Energies=	-693.407573
Sum of electronic and thermal Enthalpies=	-693.406629
Sum of electronic and thermal Free Energies=	-693.459698



Charge = 0 Multiplicity = 2

C,0,0.5630121526,0.9673275719,-0.4189658709  
C,0,0.3209334478,1.1441744906,1.0561309153  
C,0,1.5623024066,0.7413619337,1.7364168877  
C,0,2.5155626077,0.3236116757,0.7769485476  
C,0,1.9578562286,0.4609409409,-0.5363469755  
H,0,0.158505511,1.6460817797,-1.1648403755  
H,0,-0.3108521008,1.9291894672,1.4614827831  
H,0,1.6956324702,0.7313435484,2.8120014808  
C,0,-0.4704777845,0.0371803383,0.2565263318  
C,0,-1.9218339889,0.2302774761,0.0053223189  
C,0,-2.5453706764,-1.0404392876,0.0714040292  
C,0,-1.5104098923,-2.0347024743,0.3577356924  
C,0,-0.3095107585,-1.4228247224,0.4644383034  
H,0,-1.6950849739,-3.098348659,0.4652516015  
H,0,0.6403576043,-1.8989734656,0.6709153724  
H,0,4.2628192363,-0.2953562945,1.9155152436  
C,0,3.829526987,-0.1760014137,0.9258630331  
H,0,5.5787192932,-0.8659191702,-0.1095018169  
C,0,4.5626473844,-0.4938252376,-0.2118577173  
H,0,4.6066462496,-0.5898054319,-2.368799975  
C,0,4.0120042551,-0.3382933418,-1.495073659  
H,0,2.277700937,0.2397284948,-2.6555449729  
C,0,2.7006857312,0.1336296535,-1.659683303  
H,0,-4.4061939177,-2.1315532797,-0.0798622466

C,0,-3.9205908162,-1.1598335623,-0.1278284482  
H,0,-5.7402706722,-0.0861261581,-0.549984895  
C,0,-4.6677636148,-0.0072133031,-0.3925030747  
H,0,-4.6464529009,2.1309818102,-0.6640690167  
C,0,-4.0501617453,1.246375845,-0.4570679481  
H,0,-2.201035424,2.353833783,-0.3108797483  
C,0,-2.6694624161,1.3730986227,-0.2579813373

E(UB3LYP) = -693.671633038 A.U.

S\*\*2 = 0.7770

Zero-point correction=	0.249415 (Hartree/Particle)
Thermal correction to Energy=	0.262065
Thermal correction to Enthalpy=	0.263009
Thermal correction to Gibbs Free Energy=	0.209624
Sum of electronic and zero-point Energies=	-693.422218
Sum of electronic and thermal Energies=	-693.409569
Sum of electronic and thermal Enthalpies=	-693.408624
Sum of electronic and thermal Free Energies=	-693.462009

## TS10

Charge = 0 Multiplicity = 2

C,0,-0.5885277871,1.3407670101,-0.9959813476  
C,0,-0.2477708587,1.9126037518,0.8566293302  
C,0,-1.3438876242,1.2868051092,1.4484753842  
C,0,-2.0740913529,0.3399859422,0.6387818444  
C,0,-1.712116836,0.4365494418,-0.7363267507  
H,0,-0.6136103546,2.0465144666,-1.8216195833  
H,0,0.0874841886,2.8844750326,1.210199009  
H,0,-1.74665473,1.6515475391,2.3895852117  
C,0,0.6575834106,1.2320720801,-0.180576895  
C,0,1.3608110552,-0.0831019412,0.1176531764  
C,0,2.7367530079,0.0814981758,-0.1662950665  
C,0,2.9556216268,1.452546378,-0.6350400255  
C,0,1.7871110457,2.116358358,-0.6450109651  
H,0,3.9218058447,1.8526356278,-0.9249225425  
H,0,1.6279880462,3.1476402003,-0.9433513922  
H,0,4.6942998125,-0.8341670114,-0.2032389451  
C,0,3.6377204629,-0.9664417603,0.0170273095  
H,0,3.8445194127,-3.0196226942,0.6395824569  
C,0,3.1571059421,-2.1910018179,0.4902891982  
H,0,1.4381128579,-3.3118007304,1.1422879626  
C,0,1.7994455598,-2.3553227205,0.7738099737  
H,0,-0.1576945462,-1.4517322574,0.8197489262  
C,0,0.8910025157,-1.3024645198,0.5910528703  
H,0,-2.1726836661,-0.1935491859,-2.745058389

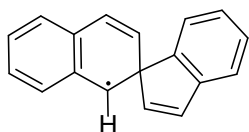
C,0,-2.4301152992,-0.2788909522,-1.6921965114  
 H,0,-4.0276462028,-1.6844435919,-2.0392509243  
 C,0,-3.4748243276,-1.1225247129,-1.291448029  
 H,0,-4.6233479075,-1.8983137141,0.360851725  
 C,0,-3.8096508271,-1.2436118781,0.0608762336  
 H,0,-3.4019957999,-0.5774311421,2.0745968487  
 C,0,-3.1180964994,-0.5090585633,1.0269879167

E(UB+HF-LYP) = -693.637431209 A.U.

S\*\*2 = 0.7805

Imaginary Mode = -655.5003

Zero-point correction=	0.247717 (Hartree/Particle)
Thermal correction to Energy=	0.260239
Thermal correction to Enthalpy=	0.261183
Thermal correction to Gibbs Free Energy=	0.208135
Sum of electronic and zero-point Energies=	-693.389714
Sum of electronic and thermal Energies=	-693.377192
Sum of electronic and thermal Enthalpies=	-693.376248
Sum of electronic and thermal Free Energies=	-693.429296



26

Charge = 0 Multiplicity = 2

H,0,-4.0958917451,1.8070488318,-0.8439082285  
 C,0,-3.3905228557,0.982637115,-0.9064801075  
 C,0,-1.56090297,-1.1709642896,-1.0699083416  
 C,0,-2.2466301944,0.9559378766,-0.1044690484  
 C,0,-3.6116980477,-0.0760950306,-1.7955148251  
 C,0,-2.7070024862,-1.1415859399,-1.878481791  
 C,0,-1.3377586288,-0.1189431642,-0.191244454  
 H,0,-4.4945465659,-0.0712510144,-2.4284946503  
 H,0,-2.8941042993,-1.9530730459,-2.5758280196  
 H,0,-0.8611552565,-1.9995980135,-1.1361149717  
 C,0,-1.7447813217,1.9010711001,0.8994757695  
 H,0,-2.2420144154,2.8259245838,1.1730137994  
 C,0,-0.1916980363,0.0887796858,0.812693438  
 C,0,-0.586045712,1.4463005084,1.4142398513  
 H,0,0.0209252714,1.9238033201,2.1745452053  
 C,0,-0.27789115,-0.9604042957,1.9024719543  
 H,0,-1.2421721838,-1.0613243097,2.3913912089  
 C,0,1.1908970375,0.1424262383,0.1474493655  
 C,0,3.7211795535,0.3023973952,-1.0911532643  
 C,0,2.2503317692,-0.6994865636,0.5842335941

C,0,1.4239487333,1.0428600373,-0.8960315164  
C,0,2.6721642379,1.1303813935,-1.5160109407  
C,0,3.5097368008,-0.5984221662,-0.0567979578  
H,0,0.6147630086,1.6860046824,-1.2306734622  
H,0,2.8260567582,1.8385147713,-2.3248239443  
H,0,4.3174333594,-1.2446206973,0.2780140859  
H,0,4.6948842746,0.364601991,-1.5685365561  
C,0,0.7855144821,-1.7447651793,2.2762649064  
H,0,0.6509723606,-2.4727594628,3.072465233  
C,0,2.0405003101,-1.6359267206,1.6517634753  
H,0,2.8662339113,-2.2671416372,1.9660061927

E(UB3LYP) = -693.740857378 A.U.

S\*\*2 = 0.7817

Zero-point correction=	0.248976 (Hartree/Particle)
Thermal correction to Energy=	0.261880
Thermal correction to Enthalpy=	0.262824
Thermal correction to Gibbs Free Energy=	0.208660
Sum of electronic and zero-point Energies=	-693.491882
Sum of electronic and thermal Energies=	-693.478977
Sum of electronic and thermal Enthalpies=	-693.478033
Sum of electronic and thermal Free Energies=	-693.532198

## TS11

Charge = 0 Multiplicity = 2

C,0,-0.2239705999,-1.6277644609,0.852417785  
C,0,-0.4200452763,0.6218545768,-0.2878424212  
C,0,-1.843878486,0.4564446908,-0.3163879923  
C,0,-2.4332438041,-0.7083662591,0.2666934801  
C,0,-1.5623086683,-1.7509009574,0.8007766984  
H,0,0.3991509984,-2.435175531,1.2273348105  
H,0,-2.0357464732,-2.6702045295,1.139831226  
C,0,0.4601134258,-0.3644320942,0.4472704838  
C,0,0.4520908549,0.8256752797,1.3893343735  
C,0,1.6912472906,1.4698796129,1.3374609121  
C,0,2.5714085532,0.7429516458,0.4602065295  
C,0,1.8777935905,-0.3851284204,-0.0604124378  
H,0,1.9462736968,2.3829539974,1.8636228166  
H,0,0.0548139046,1.3358447922,-0.9503378181  
H,0,-0.3441436278,0.9970627292,2.1009288861  
H,0,4.4486138836,1.8317238635,0.4627197441  
C,0,3.9048481439,0.9714225491,0.0806600273  
H,0,5.5602670961,0.2299383974,-1.071494214  
C,0,4.5249614991,0.0686952059,-0.7818142121  
H,0,4.3415981509,-1.7361248608,-1.9509541814

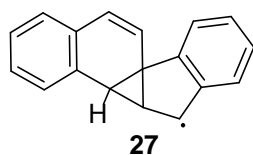
C,0,3.8361809672,-1.0457234059,-1.2813263595  
 H,0,1.9607594985,-2.1297653869,-1.3233947054  
 C,0,2.4993322576,-1.2725795986,-0.9264834848  
 H,0,-4.2663209664,-1.7478964905,0.6861279343  
 C,0,-3.8247788091,-0.8586744575,0.2411775154  
 H,0,-5.7211709159,-0.0320268571,-0.3620091676  
 C,0,-4.6430098785,0.1003437629,-0.3551732342  
 H,0,-4.6982306993,1.9724888739,-1.4329424913  
 C,0,-4.0663482838,1.2273674943,-0.9568400872  
 H,0,-2.2426219196,2.277116247,-1.4053250773  
 C,0,-2.6878448935,1.3995334512,-0.9424805684

E(UB+HF-LYP) = -693.671044222 A.U.

S\*\*2 = 0.7880

Imaginary Mode = -541.5486

Zero-point correction=	0.248647 (Hartree/Particle)
Thermal correction to Energy=	0.260960
Thermal correction to Enthalpy=	0.261904
Thermal correction to Gibbs Free Energy=	0.209432
Sum of electronic and zero-point Energies=	-693.422397
Sum of electronic and thermal Energies=	-693.410085
Sum of electronic and thermal Enthalpies=	-693.409140
Sum of electronic and thermal Free Energies=	-693.461613



Charge = 0 Multiplicity = 2

C,0,-0.2043296292,-1.7067306426,0.6973499458  
 C,0,-0.413649042,0.709623485,-0.1531835759  
 C,0,-1.869080699,0.4627554788,-0.24958094  
 C,0,-2.425365124,-0.750749646,0.2284963036  
 C,0,-1.5457918225,-1.8234173777,0.6836028204  
 H,0,0.422214167,-2.5531811784,0.9683188391  
 H,0,-2.0120774965,-2.7651534181,0.9644923965  
 C,0,0.4775538088,-0.4397263913,0.3769195404  
 C,0,0.2712288821,0.825519533,1.2233228669  
 C,0,1.5735537535,1.5122761821,1.2568174582  
 C,0,2.5149245128,0.8058354316,0.4707159422  
 C,0,1.907636801,-0.3818744664,-0.052121335  
 H,0,1.762789251,2.4345524527,1.7946780582  
 H,0,0.011646467,1.3446100027,-0.9272877822



H,0,-0.3842365105,0.8089598272,2.0897308849  
H,0,4.3392236911,1.9872511204,0.5435918943  
C,0,3.8650529722,1.0867900606,0.1616158506  
H,0,5.6238872711,0.3891853157,-0.8530539408  
C,0,4.5814688352,0.1868203524,-0.6207182537  
H,0,4.5601360144,-1.6710152876,-1.7215292201  
C,0,3.980076267,-0.9820149376,-1.1139502788  
H,0,2.1677862051,-2.1643121503,-1.2313009278  
C,0,2.6326980489,-1.26499819,-0.8346088992  
H,0,-4.2412057793,-1.8653183658,0.5340723636  
C,0,-3.816475331,-0.934940423,0.1633741557  
H,0,-5.7207399879,-0.118973619,-0.419083578  
C,0,-4.6466369434,0.0408172979,-0.3804075029  
H,0,-4.730330524,1.9812605913,-1.3257323491  
C,0,-4.0910789262,1.2185710461,-0.8892835425  
H,0,-2.2812948166,2.338113839,-1.2177390308  
C,0,-2.7128512162,1.4183667271,-0.8292448735

E(UB3LYP) = -693.682902759 A.U.

S\*\*2 = 0.7772

Zero-point correction=	0.250146 (Hartree/Particle)
Thermal correction to Energy=	0.262601
Thermal correction to Enthalpy=	0.263545
Thermal correction to Gibbs Free Energy=	0.210942
Sum of electronic and zero-point Energies=	-693.432757
Sum of electronic and thermal Energies=	-693.420302
Sum of electronic and thermal Enthalpies=	-693.419358
Sum of electronic and thermal Free Energies=	-693.471961

## TS12

Charge = 0 Multiplicity = 2

C,0,-0.1799133797,-1.6998441331,0.6900171381  
C,0,-0.3870191893,0.6518485332,-0.2293937988  
C,0,-1.865970357,0.4189324499,-0.2774661328  
C,0,-2.4159013182,-0.7838914239,0.2346779109  
C,0,-1.5355356896,-1.82959488,0.7276835589  
H,0,0.4603247759,-2.5086191057,1.0341440903  
H,0,-1.9889496589,-2.7416225453,1.1070120764  
C,0,0.4536273136,-0.502094683,0.2165980354  
C,0,0.1938143299,1.1189532547,1.1015856244  
C,0,1.5260767484,1.5675176742,1.1975573819  
C,0,2.4701149331,0.8362143903,0.3955451328  
C,0,1.9025313382,-0.3831218077,-0.0790978041  
H,0,1.8380573161,2.2524950945,1.9805856597  
H,0,-0.0068060205,1.2113637347,-1.0883264592

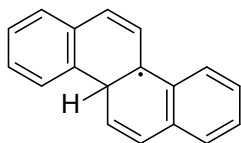
H,0,-0.5065450562,1.2216787834,1.9261140082  
 H,0,4.2677081579,2.0347048787,0.5134124031  
 C,0,3.8250902044,1.1100846937,0.150727293  
 H,0,5.6535823364,0.3887110051,-0.7245028836  
 C,0,4.6031002302,0.1801275781,-0.5394548772  
 H,0,4.6631750617,-1.7446976513,-1.5130817489  
 C,0,4.0456201334,-1.0237336854,-0.984495735  
 H,0,2.2597148471,-2.238827326,-1.1114066081  
 C,0,2.6905369242,-1.3063918387,-0.7549674434  
 H,0,-4.234000783,-1.8807112643,0.5979958011  
 C,0,-3.8113214104,-0.9595557781,0.2031374081  
 H,0,-5.7215620381,-0.1374825977,-0.3465074569  
 C,0,-4.6459622321,0.0167058514,-0.3320237907  
 H,0,-4.7418228981,1.9536509466,-1.282824565  
 C,0,-4.0969634201,1.1895356993,-0.8576120217  
 H,0,-2.2856609938,2.2940470461,-1.2361516392  
 C,0,-2.7141464459,1.3798570162,-0.8312463878

E(UB+HF-LYP) = -693.669528578 A.U.

S\*\*2 = 0.7876

Imaginary Mode = -653.6075

Zero-point correction=	0.248903 (Hartree/Particle)
Thermal correction to Energy=	0.261192
Thermal correction to Enthalpy=	0.262136
Thermal correction to Gibbs Free Energy=	0.209777
Sum of electronic and zero-point Energies=	-693.420626
Sum of electronic and thermal Energies=	-693.408336
Sum of electronic and thermal Enthalpies=	-693.407392
Sum of electronic and thermal Free Energies=	-693.459752



19

Charge = 0 Multiplicity = 2

C,0,-0.1063161629,-1.8563873184,0.1511263223  
 C,0,-0.4196352371,0.5745591822,-0.4401338526  
 C,0,-1.9106549369,0.3502649179,-0.1976945038  
 C,0,-2.4000867709,-0.9471730142,0.1027084675  
 C,0,-1.4785772447,-2.0421545052,0.2419760006  
 H,0,0.5424965728,-2.7054730376,0.3486803081  
 H,0,-1.8771132916,-3.0259447933,0.474497599  
 C,0,0.4688571248,-0.613485155,-0.1088153757

C,0,0.1287264067,1.8526445497,0.1728427761  
 C,0,1.4406824366,2.0011231608,0.406392624  
 C,0,2.3955748932,0.9269715746,0.1568378563  
 C,0,1.9057395526,-0.3897231091,-0.0928070964  
 H,0,1.8268656076,2.9397770027,0.7986486018  
 H,0,-0.3220886243,0.7182620142,-1.5402000846  
 H,0,-0.562383006,2.6651012801,0.3748128367  
 H,0,4.135550241,2.15902771,0.4257523697  
 C,0,3.7768666774,1.152611075,0.2212722314  
 H,0,5.7537123412,0.3092983299,0.0763597559  
 C,0,4.6857669852,0.1148935751,0.0312310345  
 H,0,4.9137463103,-1.9935403708,-0.3808320607  
 C,0,4.2128738437,-1.1787657861,-0.219796092  
 H,0,2.4976721394,-2.4301546496,-0.4955886637  
 C,0,2.8460975656,-1.4256580781,-0.2748754596  
 H,0,-4.1544320573,-2.1330547558,0.5093636915  
 C,0,-3.7887421948,-1.1370731486,0.270007822  
 H,0,-5.7451885325,-0.246219174,0.2623668904  
 C,0,-4.6790769479,-0.0810871189,0.1319091489  
 H,0,-4.8839941957,2.0247685334,-0.3076441143  
 C,0,-4.1963401201,1.1926283512,-0.1845302464  
 H,0,-2.468799294,2.3882031429,-0.6125261886  
 C,0,-2.8240785416,1.3954596451,-0.3482867285

E(UB3LYP) = -693.715166574 A.U.

S\*\*2 = 0.7884

Zero-point correction=	0.250739 (Hartree/Particle)
Thermal correction to Energy=	0.263320
Thermal correction to Enthalpy=	0.264264
Thermal correction to Gibbs Free Energy=	0.211048
Sum of electronic and zero-point Energies=	-693.464428
Sum of electronic and thermal Energies=	-693.451846
Sum of electronic and thermal Enthalpies=	-693.450902
Sum of electronic and thermal Free Energies=	-693.504119

### III. Spectroscopy

