Supporting Information Part 2

Conformations and CH/π Interactions in Aliphatic Alkynes and Alkenes

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1. Basis sets used in this work

Dunning TZP basis for carbon (C), ground/initial state:

```
C   0
S   6  1.00
     9471.00000         0.776000000E-03
     1398.00000         0.621800000E-02
     307.500000         0.335750000E-01
     84.5400000         0.134278000
     26.9100000         0.393668000
     9.40900000         0.544169000
S   2  1.00
     9.40900000         0.248075000
     3.50000000         0.782844000
S   1  1.00
     1.06800000          1.00000000
S   1  1.00
    0.400200000          1.00000000
S   1  1.00
    0.135100000          1.00000000
P   4  1.00
     25.3700000         0.162950000E-01
     5.77600000         0.102098000
     1.78700000         0.340228000
    0.657700000          0.668269000
P   1  1.00
    0.248000000          1.00000000
P   1  1.00
    0.910600000E-01       1.00000000
D   1  1.00
    0.626000000          1.00000000
```

Dunning TZP basis for hydrogen (H), both ground/initial and core-ionized state:

```
H 0
S   3  1.00
     74.6900000         0.253740000E-01
     11.2300000         0.189684000
     2.54600000         0.852933000
S   1  1.00
    0.713000000          1.00000000
S   1  1.00
    0.224900000          1.00000000
P   1  1.00
    0.750000000          1.00000000
```

Dunning TZP basis for carbon (C), core-ionized state:

```
S   6  0.964
     13520.0000         0.760000000E-03
     1999.00000         0.607600000E-02
     440.000000         0.328470000E-01
     120.900000         0.132396000
     38.4700000         0.393261000
     13.4600000         0.546339000
S   2   0.964
     13.4600000         0.252036000
     4.99300000         0.779385000
S   1  0.964
     1.56900000          1.00000000
S   1  0.964
    0.580000000          1.00000000
S   1  0.964
    0.192300000          1.00000000
P   4  0.964
     35.9100000         0.169160000E-01
     8.48000000         0.102200000
     2.70600000         0.338134000
    0.992100000         0.669281000
P   1  0.964
    0.372700000          1.00000000
P   1  0.964
    0.134600000          1.00000000
D   1  0.964
    0.913000000          1.00000000
```

6-311++G(3df,3dp) basis for carbon (C), ground/initial state:

```
S   6  1.00
      4563.24000         0.196665000E-02
      682.024000         0.152306000E-01
      154.973000         0.761269000E-01
      44.4553000         0.260801000
      13.0290000         0.616462000
      1.82773000         0.221006000
SP  3  1.00
      20.9642000         0.114660000         0.402487000E-01
      4.80331000         0.919999000         0.237594000
      1.45933000        -0.303068000E-02     0.815854000
 SP  1  1.00
     0.483456000          1.00000000          1.00000000
 SP  1  1.00
     0.145585000          1.00000000          1.00000000
 D   1  1.00
      2.50400000          1.00000000
```

D 1 1.00
0.626000000 1.00000000
D 1 1.00
0.156500000 1.00000000
F 1 1.00
0.800000000 1.00000000
SP 1 1.00
0.438000000E-01 1.00000000 1.00000000

6-311++G(3df,3dp) basis for carbon (H), ground/initial state:

S 3 1.00
33.8650000 0.254938000E-01
5.09479000 0.190373000
1.15879000 0.852161000
S 1 1.00
0.325840000 1.00000000
S 1 1.00
0.102741000 1.00000000
P 1 1.00
3.00000000 1.00000000
P 1 1.00
0.750000000 1.00000000
P 1 1.00
0.187500000 1.00000000
D 1 1.00
1.00000000 1.00000000
S 1 1.00
0.360000000E-01 1.00000000

Aug-cc-pVTZ basis for carbon (C), ground/initial state:

S 8 1.00
8236.00000 0.531000000E-03
1235.00000 0.410800000E-02
280.800000 0.210870000E-01
79.2700000 0.818530000E-01
25.5900000 0.234817000
8.99700000 0.434401000
3.31900000 0.346129000
0.364300000 -0.898300000E-02
S 8 1.00
8236.00000 -0.113000000E-03
1235.00000 -0.878000000E-03
280.800000 -0.454000000E-02
79.2700000 -0.181330000E-01
25.5900000 -0.557600000E-01
8.99700000 -0.126895000
3.31900000 -0.170352000
0.364300000 0.598684000

S 1 1.00
0.905900000 1.00000000
S 1 1.00
0.128500000 1.00000000
P 3 1.00
18.7100000 0.140310000E-01
4.13300000 0.868660000E-01
1.20000000 0.290216000
P 1 1.00
0.382700000 1.00000000
P 1 1.00
0.120900000 1.00000000
D 1 1.00
1.09700000 1.00000000
D 1 1.00
0.318000000 1.00000000
F 1 1.00
0.761000000 1.00000000
S 1 1.00
0.440200000E-01 1.00000000
P 1 1.00
0.356900000E-01 1.00000000
D 1 1.00
0.100000000 1.00000000
F 1 1.00
0.268000000 1.00000000

Aug-cc-pVTZ basis for carbon (H), ground/initial state:

S 3 1.00
33.8700000 0.606800000E-02
5.09500000 0.453080000E-01
1.15900000 0.202822000
S 1 1.00
0.325800000 1.00000000
S 1 1.00
0.102700000 1.00000000
P 1 1.00
1.40700000 1.00000000
P 1 1.00
0.388000000 1.00000000
D 1 1.00
1.05700000 1.00000000
S 1 1.00
0.252600000E-01 1.00000000
P 1 1.00
0.102000000 1.00000000
D 1 1.00
0.247000000 1.00000000

cc-pVQZ basis for carbon (C), ground/initial state:

```
S   9  1.00
      33980.0000         0.910000000E-04
      5089.00000         0.704000000E-03
      1157.00000         0.369300000E-02
      326.600000         0.153600000E-01
      106.100000         0.529290000E-01
      38.1100000         0.147043000
      14.7500000         0.305631000
      6.03500000         0.399345000
      2.53000000         0.217051000
S   9  1.00
      33980.0000        -0.190000000E-04
      5089.00000        -0.151000000E-03
      1157.00000        -0.785000000E-03
      326.600000        -0.332400000E-02
      106.100000        -0.115120000E-01
      38.1100000        -0.341600000E-01
      14.7500000        -0.771730000E-01
      6.03500000        -0.141493000
      2.53000000        -0.118019000
S   1  1.00
     0.735500000          1.00000000
S   1  1.00
     0.290500000          1.00000000
S   1  1.00
     0.111100000          1.00000000
P   3  1.00
      34.5100000         0.537800000E-02
      7.91500000         0.361320000E-01
      2.36800000         0.142493000
P   1  1.00
     0.813200000          1.00000000
P   1  1.00
     0.289000000          1.00000000
P   1  1.00
     0.100700000          1.00000000
D   1  1.00
      1.84800000          1.00000000
D   1  1.00
     0.649000000          1.00000000
D   1  1.00
     0.228000000          1.00000000
F   1  1.00
      1.41900000          1.00000000
F   1  1.00
     0.485000000          1.00000000
G   1  1.00
      1.01100000          1.00000000
```

cc-pVQZ basis for carbon (H), ground/initial state:

```
S   3  1.00
     82.6400000         0.200600000E-02
     12.4100000         0.153430000E-01
     2.82400000         0.755790000E-01
S   1  1.00
    0.797700000          1.00000000
S   1  1.00
    0.258100000          1.00000000
S   1  1.00
    0.898900000E-01      1.00000000
P   1  1.00
     2.29200000          1.00000000
P   1  1.00
    0.838000000          1.00000000
P   1  1.00
    0.292000000          1.00000000
D   1  1.00
     2.06200000          1.00000000
D   1  1.00
    0.662000000          1.00000000
F   1  1.00
     1.39700000          1.00000000
```

2. Optimized geometries from B3LYP/TZP calculations

Anti-4-methyl-1-pentyne, ground state:

```
C
C                1    rc1c2
X                1    1.      2     90.
X                2    1.      1     90.      3     0.       0
H                1    rc1h5   3     90.      2     d9       0
C                2    rc6c2   4     90.      1     d10      0
H                6    rc6h7   2    ac2c6h7  4    d1       0
H                6    rc6h8   2    ac2c6h8  4    d8       0
C                6    rc6c9   2    ac2c6c9  4    d2       0
H                9    rc9h10  6    ac6c9h10 2    d3       0
C                9    rc9c12  6    ac6c9c12 2    d4       0
H                11   rc12h13  9    ac9c12h13 6    d5       0
H                11   rc12h14  9    ac9c12h14 6    d11      0
H                11   rc12h15  9    ac9c12h15 6    d6       0
C                9    rc9c13  6    ac6c9c13 2    d7       0
H                15   rc12h16  9    ac9c12h16 6    d12      0
H                15   rc12h17  9    ac9c12h17 6    d13      0
H                15   rc12h18  9    ac9c12h18 6    d14      0
     Variables:
   rc1c2        1.2048
   rc6c2        1.461
   rc1h5        1.0632
   rc6h7        1.0961
   rc6c9        1.5491
  rc9h10        1.0946
  rc9c12        1.5332
  rc12h13       1.0934
  rc12h15       1.0927
  ac2c6h7     109.0989
  ac2c6c9     114.2921
 ac6c9h10     107.3367
 ac6c9c12     109.7474
 ac9c12h13    111.6214
 ac9c12h15    110.9422
    d1         96.5792
    d2        -25.9582
    d3        -55.8188
    d4        186.4538
    d5         58.4662
    d6        178.6284
    d9        180.06
    d10       179.5636
  rc9c13        1.5324
 ac6c9c13     111.5438
    d7         62.7427
  rc12h14       1.0942
```

d14 182.2668
d13 62.7077
d12 -57.4857
d11 -61.8303
rc6h8 1.0955
ac2c6h8 108.5416
rc12h16 1.0921
rc12h18 1.0929
rc12h17 1.0942
ac9c12h14 111.0284
ac9c12h16 111.4386
ac9c12h17 110.9109
ac9c12h18 110.8508
d8 -148.05

Anti-4-methyl-1-pentyne, core-ionized state, C1*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14
Variables:
rc1c2 1.1669
rc6c2 1.4245
rc1h5 1.0282
rc6h7 1.098
rc6c9 1.5801
rc9h10 1.0931
rc9c12 1.5318
rc12h13 1.0921
rc12h15 1.0914
ac2c6h7 107.4584
ac2c6c9 112.8375
ac6c9h10 106.9706
ac6c9c12 107.4139
ac9c12h13 112.1091

ac9c12h15 109.2558
d1 45.237
d2 -77.1331
d3 -56.1728
d4 186.9793
d5 59.5099
d6 178.7307
d9 179.6015
d10 178.2207
rc9c13 1.5299
ac6c9c13 111.1156
d7 63.5477
rc12h14 1.0927
d14 180.3584
d13 61.5196
d12 -60.6559
d11 -62.398
rc6h8 1.0981
ac2c6h8 106.7825
rc12h16 1.0939
rc12h18 1.0913
rc12h17 1.0928
ac9c12h14 111.4378
ac9c12h16 112.8504
ac9c12h17 111.4644
ac9c12h18 109.6054
d8 -199.5172

Anti-4-methyl-1-pentyne, core-ionized state, C2*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14
Variables:
rc1c2 1.1576

rc6c2 1.4479
rc1h5 1.0763
rc6h7 1.0942
rc6c9 1.5554
rc9h10 1.094
rc9c12 1.5341
rc12h13 1.0923
rc12h15 1.0911
ac2c6h7 106.7441
ac2c6c9 112.6997
ac6c9h10 107.2115
ac6c9c12 107.3322
ac9c12h13 112.0551
ac9c12h15 109.5313
d1 42.1491
d2 -80.1388
d3 -58.0812
d4 185.2661
d5 58.5576
d6 177.8811
d9 179.7319
d10 177.9487
rc9c13 1.5306
ac6c9c13 111.8095
d7 61.9996
rc12h14 1.0927
d14 179.9886
d13 61.0849
d12 -61.0129
d11 -63.1836
rc6h8 1.0937
ac2c6h8 106.4442
rc12h16 1.0935
rc12h18 1.0912
rc12h17 1.093
ac9c12h14 111.4511
ac9c12h16 112.8913
ac9c12h17 111.3874
ac9c12h18 109.7857
d8 -202.4573

Anti-4-methyl-1-pentyne, core-ionized state, C3*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1

H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14

Variables:

rc1c2	1.195
rc6c2	1.4062
rc1h5	1.068
rc6h7	1.0397
rc6c9	1.5919
rc9h10	1.09
rc9c12	1.5225
rc12h13	1.0929
rc12h15	1.0909
ac2c6h7	110.7752
ac2c6c9	115.3321
ac6c9h10	103.0216
ac6c9c12	107.5905
ac9c12h13	112.5212
ac9c12h15	108.3835
d1	74.043
d2	-47.4028
d3	-53.5438
d4	189.0163
d5	58.912
d6	177.2437
d9	179.9875
d10	179.6063
rc9c13	1.5197
ac6c9c13	109.0118
d7	64.3485
rc12h14	1.0927
d14	183.8292
d13	65.5862
d12	-57.6306
d11	-64.5403
rc6h8	1.0392
ac2c6h8	110.488
rc12h16	1.0906
rc12h18	1.0911
rc12h17	1.0927
ac9c12h14	111.9871
ac9c12h16	112.295

ac9c12h17 111.801
ac9c12h18 108.2128
d8 -168.6086

Anti-4-methyl-1-pentyne, core-ionized state, C4*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14
Variables:
rc1c2 1.2013
rc6c2 1.4522
rc1h5 1.0671
rc6h7 1.0922
rc6c9 1.5317
rc9h10 1.0334
rc9c12 1.508
rc12h13 1.0884
rc12h15 1.0881
ac2c6h7 111.716
ac2c6c9 112.1229
ac6c9h10 106.3292
ac6c9c12 111.1222
ac9c12h13 109.4497
ac9c12h15 109.179
d1 6.2205
d2 -113.7134
d3 -53.4695
d4 189.3566
d5 58.0638
d6 178.2471
d9 179.4324
d10 181.3869
rc9c13 1.5102
ac6c9c13 112.0815

d7 63.4324
rc12h14 1.0884
d14 184.6409
d13 64.9066
d12 -55.0571
d11 -62.0744
rc6h8 1.092
ac2c6h8 110.8789
rc12h16 1.0876
rc12h18 1.0881
rc12h17 1.0884
ac9c12h14 108.8437
ac9c12h16 109.0381
ac9c12h17 108.6951
ac9c12h18 109.0344
d8 -233.2958

Anti-4-methyl-1-pentyne, core-ionized state, C5,a*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14
Variables:
rc1c2 1.2017
rc6c2 1.4568
rc1h5 1.0659
rc6h7 1.0968
rc6c9 1.5422
rc9h10 1.0905
rc9c12 1.552
rc12h13 1.0356
rc12h15 1.0354
ac2c6h7 109.6991
ac2c6c9 111.1816
ac6c9h10 109.4374

ac6c9c12 108.0259
ac9c12h13 111.3516
ac9c12h15 110.5878
d1 56.4663
d2 -65.2339
d3 -59.4174
d4 186.8889
d5 57.6881
d6 178.1098
d9 179.5384
d10 179.7129
rc9c13 1.5225
ac6c9c13 114.3806
d7 65.355
rc12h14 1.0361
d14 181.0447
d13 58.2923
d12 -60.2826
d11 -62.5355
rc6h8 1.097
ac2c6h8 108.9538
rc12h16 1.0899
rc12h18 1.0924
rc12h17 1.0929
ac9c12h14 110.4345
ac9c12h16 108.6059
ac9c12h17 111.7769
ac9c12h18 111.9744
d8 -186.6424

Anti-4-methyl-1-pentyne, core-ionized state, C5,b*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d8
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d11
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c13 6 ac6c9c13 2 d7
H 15 rc12h16 9 ac9c12h16 6 d12
H 15 rc12h17 9 ac9c12h17 6 d13
H 15 rc12h18 9 ac9c12h18 6 d14

Variables:

rc1c2	1.2044
rc6c2	1.4597
rc1h5	1.0669
rc6h7	1.0954
rc6c9	1.5434
rc9h10	1.0906
rc9c12	1.522
rc12h13	1.0908
rc12h15	1.0921
ac2c6h7	110.3168
ac2c6c9	111.7685
ac6c9h10	108.8653
ac6c9c12	113.8906
ac9c12h13	108.9941
ac9c12h15	111.9434
d1	6.0368
d2	-117.1886
d3	-63.71
d4	172.1192
d5	60.8335
d6	179.3566
d9	176.4931
d10	175.6307
rc9c13	1.543
ac6c9c13	107.9886
d7	49.1037
rc12h14	1.0926
d14	193.8105
d13	72.4088
d12	-45.8482
d11	-58.0984
rc6h8	1.0935
ac2c6h8	110.4031
rc12h16	1.0445
rc12h18	1.0343
rc12h17	1.0354
ac9c12h14	111.8747
ac9c12h16	107.8231
ac9c12h17	111.2549
ac9c12h18	111.9057
d8	-236.7179

Gauche-4-methyl-1-pentyne, ground state:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9

C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6
Variables:

rc1c2	1.2048
rc6c2	1.4619
rc1h5	1.0632
rc6h7	1.0955
rc6h8	1.0955
rc6c9	1.5515
rc9h10	1.0955
rc9c12	1.5328
rc12h13	1.093
rc12h14	1.0934
rc12h15	1.0928
ac2c6h7	108.6003
ac2c6h8	108.6265
ac2c6c9	114.7025
ac6c9h10	105.709
ac6c9c12	111.481
ac9c12h13	110.9147
ac9c12h14	111.5499
ac9c12h15	110.8195
d1	114.7889
d2	-7.5807
d3	180.0
d4	-62.694
d5	60.5218
d6	179.9998
d9	179.9575
d10	180.123
d11	-129.9603
d13	-59.6022

Gauche-4-methyl-1-pentyne, core-ionized state, C1*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0

H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6
Variables:

rc1c2	1.1666
rc6c2	1.4263
rc1h5	1.0282
rc6h7	1.0983
rc6h8	1.0983
rc6c9	1.5773
rc9h10	1.0928
rc9c12	1.5305
rc12h13	1.0948
rc12h14	1.0921
rc12h15	1.091
ac2c6h7	106.5631
ac2c6h8	106.5007
ac2c6c9	113.5352
ac6c9h10	103.0076
ac6c9c12	111.0121
ac9c12h13	112.0268
ac9c12h14	112.2229
ac9c12h15	109.6709
d1	108.0743
d2	-14.587
d3	180.0008
d4	-63.3877
d5	62.03
d6	180.0006
d9	179.8651
d10	179.8861
d11	-137.2047
d13	-60.0793

Gauche-4-methyl-1-pentyne, core-ionized state, C2*:

C
C 1 rc1c2
X 1 1.0 2 90.0

X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6
Variables:

rc1c2	1.1574
rc6c2	1.4488
rc1h5	1.0763
rc6h7	1.0939
rc6h8	1.0939
rc6c9	1.5555
rc9h10	1.094
rc9c12	1.5315
rc12h13	1.0943
rc12h14	1.0922
rc12h15	1.0909
ac2c6h7	106.2832
ac2c6h8	106.2888
ac2c6c9	112.9794
ac6c9h10	102.993
ac6c9c12	111.4918
ac9c12h13	112.0055
ac9c12h14	112.1481
ac9c12h15	109.8799
d1	117.9467
d2	-4.4306
d3	179.9999
d4	-63.5866
d5	62.0325
d6	180.0001
d9	179.9803
d10	180.0299
d11	-126.808
d13	-59.9636

Gauche-4-methyl-1-pentyne, core-ionized state, C3*:

C
C 1 rc1c2

X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6

Variables:

rc1c2	1.195
rc6c2	1.4065
rc1h5	1.068
rc6h7	1.0391
rc6h8	1.0391
rc6c9	1.5985
rc9h10	1.0917
rc9c12	1.5198
rc12h13	1.0912
rc12h14	1.0923
rc12h15	1.0909
ac2c6h7	110.2662
ac2c6h8	110.2843
ac2c6c9	115.8813
ac6c9h10	102.1853
ac6c9c12	108.7558
ac9c12h13	111.6908
ac9c12h14	112.4636
ac9c12h15	108.2148
d1	104.2133
d2	-17.1882
d3	179.9996
d4	-62.8908
d5	62.0167
d6	179.9996
d9	179.9667
d10	180.2
d11	-138.5948
d13	-61.0797

Gauche-4-methyl-1-pentyne, core-ionized state, C4*:

C

C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6

Variables:

rc1c2	1.2014
rc6c2	1.4517
rc1h5	1.0671
rc6h7	1.0924
rc6h8	1.0924
rc6c9	1.5341
rc9h10	1.0325
rc9c12	1.5104
rc12h13	1.0876
rc12h14	1.0885
rc12h15	1.0879
ac2c6h7	111.027
ac2c6h8	111.0248
ac2c6c9	112.6818
ac6c9h10	105.9271
ac6c9c12	111.925
ac9c12h13	108.5059
ac9c12h14	109.3189
ac9c12h15	109.055
d1	29.5648
d2	-90.3947
d3	179.9999
d4	-63.2551
d5	60.2815
d6	180.0
d9	179.608
d10	182.4879
d11	-210.3541
d13	-59.5272

Gauche-4-methyl-1-pentyne, core-ionized state, C5*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h8 2 ac2c6h8 4 d11
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 11 rc12h13 9 ac9c12h13 6 d5
H 11 rc12h14 9 ac9c12h14 6 d13
H 11 rc12h15 9 ac9c12h15 6 d6
C 9 rc9c12 6 ac6c9c12 2 -d4
H 15 rc12h13 9 ac9c12h13 6 -d5
H 15 rc12h14 9 ac9c12h14 6 -d13
H 15 rc12h15 9 ac9c12h15 6 d6
Variables:

rc1c2	1.2037
rc6c2	1.4603
rc1h5	1.0665
rc6h7	1.0934
rc6h8	1.096
rc6c9	1.5423
rc9h10	1.0906
rc9c12	1.5323
rc12h13	1.0647
rc12h14	1.0617
rc12h15	1.0625
ac2c6h7	110.4404
ac2c6h8	110.0559
ac2c6c9	112.3126
ac6c9h10	109.1942
ac6c9c12	110.9689
ac9c12h13	110.0975
ac9c12h14	110.2347
ac9c12h15	111.704
d1	74.4089
d2	-44.5255
d3	183.4445
d4	-60.7304
d5	58.5596
d6	179.3516
d9	177.4071
d10	177.1391
d11	-168.8629
d13	-60.1403

Anti-2-hexyne, ground state:

C
C,1,rc1c2
X,1,1.,2,90.
X,2,1.,1,90.,3,0.,0
C,1,rc1c5,3,90.,2,d5,0
C,2,rc2c6,4,90.,1,d6,0
H,5,rc5h7,1,ac1c5h7,3,d1,0
H,5,rc5h8,1,ac1c5h8,3,d11,0
H,5,rc5h9,1,ac1c5h9,3,d2,0
H,6,rc6h10,2,ac2c6h10,4,d3,0
H,6,rc6h11,2,ac2c6h11,4,d12,0
C,6,rc6c12,2,ac12c6c2,4,d4,0
H,12,rc12h13,6,ac6c12h13,2,d7,0
H,12,rc12h14,6,ac6c12h14,2,d13,0
C,12,rc12c15,6,ac15c12c6,2,d8,0
H,15,rc15h16,12,ac12c15h16,6,d9,0
H,15,rc15h17,12,ac12c15h17,6,d14,0
H,15,rc15h18,12,ac12c15h18,6,d10,0

Variables:

rc1c2	1.2061
rc1c5	1.4598
rc2c6	1.4628
rc5h7	1.0931
rc5h8	1.0932
rc5h9	1.093
rc6h10	1.0957
rc6h11	1.0957
rc6c12	1.5423
rc12h13	1.0931
rc12h14	1.0931
rc12c15	1.5301
rc15h16	1.0934
rc15h17	1.0934
rc15h18	1.0926
ac1c5h7	111.2156
ac1c5h8	111.2043
ac1c5h9	111.1407
ac2c6h10	109.332
ac2c6h11	109.308
ac12c6c2	113.436
ac6c12h13	108.8804
ac6c12h14	108.882
ac15c12c6	112.2434
ac12c15h16	111.3877
ac12c15h17	111.3871
ac12c15h18	111.186
d1	213.0149
d2	93.0385
d3	-41.0417

d4	81.174
d5	180.1796
d6	180.9609
d7	57.7258
d8	179.9881
d9	60.0146
d10	179.9975
d11	-26.9218
d12	-156.6218
d13	-57.7504
d14	-60.0203

Anti-2-hexyne, core-ionized state, C1*:

6	0.559165	-0.001133	-1.828814
6	0.546213	-0.005917	-0.628309
6	0.594096	0.004403	-3.244852
6	0.498489	-0.011009	0.825633
1	0.193170	-0.869011	-3.651799
1	0.052280	0.799705	-3.648755
1	1.567132	0.087109	-3.613072
1	1.059181	0.856431	1.188953
1	1.031984	-0.898369	1.181843
6	-0.943588	0.008781	1.388786
1	-1.487101	-0.859110	1.008018
1	-1.460291	0.896062	1.015419
6	-0.940711	0.002346	2.918039
1	-0.424099	0.876041	3.321744
1	-0.451593	-0.890347	3.314370
1	-1.962649	0.016659	3.300381

Anti-2-hexyne, core-ionized state, C2*:

6	0.565045	-0.000167	-1.784965
6	0.560445	-0.004229	-0.618788
6	0.578539	0.003309	-3.229719
6	0.510584	-0.010605	0.816360
1	0.144373	-0.927746	-3.595172
1	-0.006144	0.849186	-3.592536
1	1.607742	0.091201	-3.579073
1	1.075223	0.861876	1.166941
1	1.048471	-0.903375	1.157667
6	-0.951384	0.009243	1.363242
1	-1.485548	-0.860878	0.977452
1	-1.457768	0.899739	0.986563
6	-0.941847	0.001155	2.892090
1	-0.430285	0.876634	3.296990
1	-0.456984	-0.893533	3.287748
1	-1.967372	0.014665	3.264098

Anti-2-hexyne, core-ionized state, C3*:

6	0.563776	-0.000455	-1.788842
6	0.559529	-0.004771	-0.624813
6	0.574739	0.003909	-3.224757
6	0.507866	-0.010894	0.828085
1	0.139265	-0.928809	-3.595740
1	-0.011633	0.851626	-3.591929
1	1.605583	0.092041	-3.580995
1	1.068853	0.861793	1.171623
1	1.041536	-0.903841	1.163071
6	-0.938920	0.008674	1.359609
1	-1.472929	-0.862258	0.973011
1	-1.446302	0.898840	0.981012
6	-0.943453	0.001847	2.889630
1	-0.434519	0.877216	3.298517
1	-0.460819	-0.891920	3.290542
1	-1.970257	0.015452	3.257412

Anti-2-hexyne, core-ionized state, C4*:

6	1.893341	0.070971	-0.001110
6	0.726166	0.348314	-0.001956
6	3.306961	-0.262377	0.001319
6	-0.646923	0.669282	0.000196
1	3.579393	-0.759376	0.934843
1	3.542539	-0.930524	-0.829900
1	3.910826	0.642055	-0.099274
1	-0.888757	1.252125	-0.826119
1	-0.886630	1.248883	0.829393
6	-1.603571	-0.559733	-0.001354
1	-1.332526	-1.136202	0.881049
1	-1.334569	-1.132112	-0.887060
6	-3.056074	-0.116943	0.001382
1	-3.312773	0.464512	-0.886638
1	-3.310393	0.461022	0.892361
1	-3.686510	-1.007469	0.000480

Anti-2-hexyne, core-ionized state, C5*:

6	1.895997	0.051601	0.000277
6	0.726440	0.344456	-0.000414
6	3.311450	-0.280591	0.000455
6	-0.669384	0.732303	-0.000059
1	3.597586	-0.772526	0.932496
1	3.557128	-0.942899	-0.832547
1	3.908214	0.628918	-0.102002
1	-0.938319	1.315562	-0.883262
1	-0.937923	1.315026	0.883655
6	-1.585322	-0.504067	-0.000357

1	-1.341612	-1.078929	0.824484
1	-1.342248	-1.078149	-0.825936
6	-3.059664	-0.186324	0.000352
1	-3.296835	0.391330	-0.890321
1	-3.295736	0.392126	0.890805
1	-3.627356	-1.114730	0.001107

Anti-2-hexyne, core-ionized state, C6*:

6	1.888580	0.064166	-0.000014
6	0.723883	0.373207	-0.000811
6	3.301426	-0.289004	0.000451
6	-0.686978	0.736364	0.000026
1	3.579348	-0.787696	0.931588
1	3.537288	-0.958145	-0.830021
1	3.918427	0.606549	-0.101105
1	-0.919851	1.347125	-0.880714
1	-0.918958	1.345547	0.882156
6	-1.549581	-0.532464	-0.000465
1	-1.366924	-1.139879	0.884176
1	-1.367935	-1.138874	-0.886016
6	-3.049224	-0.183141	0.000462
1	-3.298837	0.374808	-0.836134
1	-3.297932	0.374320	0.837652
1	-3.633258	-1.038512	0.000529

Gauche-2-hexyne, ground state:

```
 c
 c   1 cc2
xx   1 xxc3      2 xxcc3
xx   2 xxc4      1 xxcc4      3 dih4
 c   1 cc5       3 ccxx5      2 dih5
 c   2 cc6       4 ccxx6      1 dih6
 h   5 hc7       1 hcc7       3 dih7
 h   5 hc8       1 hcc8       3 dih8
 h   5 hc9       1 hcc9       3 dih9
 h   6 hc10      2 hcc10      4 dih10
 h   6 hc11      2 hcc11      4 dih11
 c   6 cc12      2 ccc12      4 dih12
 h  12 hc13      6 hcc13      2 dih13
 h  12 hc14      6 hcc14      2 dih14
 c  12 cc15      6 ccc15      2 dih15
 h  15 hc16     12 hcc16      6 dih16
 h  15 hc17     12 hcc17      6 dih17
 h  15 hc18     12 hcc18      6 dih18

      cc2       1.2061
     xxc3       1.0
     xxcc3      89.8888
```

xxc4	1.0
xxcc4	90.2772
dih4	-5.9833
cc5	1.4598
ccxx5	89.8567
dih5	179.815
cc6	1.4639
ccxx6	90.2697
dih6	180.2577
hc7	1.093
hcc7	111.2319
dih7	98.8526
hc8	1.0933
hcc8	111.1726
dih8	-141.11
hc9	1.093
hcc9	111.129
dih9	-21.1879
hc10	1.0953
hcc10	108.8943
dih10	38.1694
hc11	1.0957
hcc11	109.1631
dih11	-77.3223
cc12	1.5437
ccc12	113.8832
dih12	160.2499
hc13	1.0933
hcc13	108.8782
dih13	-58.7964
hc14	1.0942
hcc14	107.9546
dih14	185.802
cc15	1.5296
ccc15	113.477
dih15	63.9691
hc16	1.0934
hcc16	111.2479
dih16	59.9757
hc17	1.092
hcc17	111.0954
dih17	-59.931
hc18	1.0927
hcc18	111.0546
dih18	179.9383

Gauche-2-hexyne, core-ionized state, C1*:

6	1.657684	-0.081308	-0.021273
6	0.552382	-0.538432	-0.124802

6	2.969114	0.443170	0.086411
6	-0.791516	-1.088899	-0.230003
1	3.279037	0.912046	-0.792986
1	3.047893	1.152183	0.848184
1	3.672790	-0.299078	0.294192
1	-0.773730	-2.092579	0.207250
1	-1.024635	-1.212747	-1.292653
6	-1.875192	-0.223212	0.458495
1	-1.629060	-0.117163	1.517544
1	-2.804566	-0.795038	0.412886
6	-2.074141	1.146080	-0.190449
1	-2.358029	1.052927	-1.241333
1	-1.170722	1.759146	-0.139997
1	-2.868969	1.695914	0.316641

Gauche-2-hexyne, core-ionized state, C2*:

6	1.617520	-0.097088	-0.027398
6	0.548422	-0.551811	-0.127112
6	2.944197	0.462572	0.091030
6	-0.776367	-1.100020	-0.227762
1	3.217086	0.941801	-0.849597
1	2.953589	1.198614	0.895481
1	3.651897	-0.336003	0.315641
1	-0.737143	-2.102657	0.216123
1	-0.993201	-1.224053	-1.295820
6	-1.856387	-0.213052	0.464876
1	-1.607699	-0.111949	1.522779
1	-2.778725	-0.794527	0.413687
6	-2.043566	1.150572	-0.196678
1	-2.320368	1.054486	-1.248596
1	-1.144567	1.769927	-0.135758
1	-2.843791	1.697321	0.304314

Gauche-2-hexyne, core-ionized state, C3*:

6	1.612891	-0.103093	-0.026289
6	0.545813	-0.557934	-0.122042
6	2.930949	0.455026	0.088998
6	-0.798715	-1.105982	-0.225040
1	3.210589	0.928074	-0.857157
1	2.943045	1.202040	0.888418
1	3.644213	-0.341006	0.323278
1	-0.767870	-2.099857	0.228088
1	-1.007721	-1.227492	-1.290967
6	-1.853990	-0.211138	0.453014
1	-1.620557	-0.125171	1.516716
1	-2.791876	-0.767414	0.385130
6	-2.009085	1.165450	-0.191621
1	-2.271311	1.087297	-1.249028

1	-1.100033	1.766880	-0.110084
1	-2.805657	1.722677	0.303486

Gauche-2-hexyne, core-ionized state, C4*:

6	1.642945	-0.091606	-0.027182
6	0.527565	-0.522715	-0.123741
6	2.992266	0.433136	0.089485
6	-0.772889	-1.058018	-0.236715
1	3.289224	0.930683	-0.836203
1	3.052187	1.155233	0.906811
1	3.698134	-0.375733	0.290053
1	-0.801699	-2.017390	0.161916
1	-1.036902	-1.159185	-1.237304
6	-1.895889	-0.226579	0.459301
1	-1.597804	-0.161280	1.504144
1	-2.794839	-0.838782	0.382186
6	-2.065457	1.134291	-0.187771
1	-2.363912	1.056379	-1.235162
1	-1.157334	1.733213	-0.117668
1	-2.858308	1.665812	0.340966

Gauche-2-hexyne, core-ionized state, C5*:

6	-1.642269	-0.082431	0.021713
6	-0.517859	-0.510134	0.102236
6	-3.002751	0.421393	-0.076940
6	0.803814	-1.088180	0.232504
1	-3.313542	0.890065	0.859041
1	-3.083553	1.161690	-0.876474
1	-3.693923	-0.394434	-0.300351
1	0.863727	-2.071814	-0.239482
1	1.107891	-1.194597	1.276116
6	1.875553	-0.212668	-0.444942
1	1.608231	-0.095535	-1.437386
1	2.773794	-0.724448	-0.436463
6	2.057553	1.146495	0.188967
1	2.387902	1.012291	1.216708
1	1.101869	1.664232	0.169543
1	2.803359	1.705706	-0.372485

Gauche-2-hexyne, core-ionized state, C6*:

6	-1.544467	-0.130578	0.016482
6	-0.434375	-0.600637	0.095283
6	-2.914667	0.357910	-0.082387
6	0.926275	-1.124954	0.196544
1	-3.268067	0.737480	0.878584
1	-2.999363	1.157594	-0.821712
1	-3.577008	-0.454098	-0.390942

1	1.025177	-2.064676	-0.354105
1	1.174145	-1.352561	1.238582
6	1.946544	-0.136995	-0.392916
1	1.825137	-0.048262	-1.471134
1	2.974852	-0.416704	-0.170156
6	1.692813	1.254276	0.185539
1	1.984163	1.318870	1.176764
1	0.657155	1.406780	0.149421
1	2.171072	2.001441	-0.346572

AA-1-hexyne, ground state:

```
C
C              1    rc1c2
X              1    1.       2     90.
X              2    1.       1     90.      3     0.       0
H              1    rc1h5    3     90.      2     d9       0
C              2    rc6c2    4     90.      1     d10      0
H              6    rc6h7    2     ac2c6h7  4     d1       0
H              6    rc6h7    2     ac2c6h7  4     -d1      0
C              6    rc6c9    2     ac2c6c9  4     d2       0
H              9    rc9h10   6     ac6c9h10 2     d3       0
H              9    rc9h10   6     ac6c9h10 2     -d3      0
C              9    rc9c12   6     ac6c9c12 2     d4       0
H              12   rc12h13  9     ac9c12h13 6    d5       0
H              12   rc12h13  9     ac9c12h13 6    -d5      0
C              12   rc12c15  9     ac9c12c15 6    d6       0
H              15   rc15h16  12    ac12c15h16 9   d7       0
H              15   rc15h16  12    ac12c15h16 9   -d7      0
H              15   rc15h18  12    ac12c15h18 9   d8       0
 Variables:
 rc1c2        1.2047
 rc6c2        1.461
 rc1h5        1.0632
 rc6h7        1.0953
 rc6c9        1.5418
 rc9h10       1.0939
 rc9c12       1.5321
 rc12h13      1.0954
 rc12c15      1.5312
 rc15h16      1.0931
 rc15h18      1.0927
 ac2c6h7     108.9534
 ac2c6c9     113.3284
 ac6c9h10    109.0141
 ac6c9c12    112.5109
 ac9c12h13    109.368
 ac9c12c15    112.7564
 ac12c15h16   111.2747
 ac12c15h18   111.3812
```

d1 122.3075
d2 0.
d3 57.77
d4 180.
d5 57.8406
d6 180.
d7 59.9124
d8 180.
d9 180.
d10 180.

AA-1-hexyne, core-ionized state, C1*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.1666
rc6c2 1.4258
rc1h5 1.0284
rc6h7 1.0981
rc6c9 1.5663
rc9h10 1.092
rc9c12 1.5343
rc12h13 1.0944
rc12c15 1.5308
rc15h16 1.0921
rc15h18 1.0913
ac2c6h7 106.9925
ac2c6c9 112.5539
ac6c9h10 108.9814
ac6c9c12 110.0218
ac9c12h13 109.4083
ac9c12c15 111.4271
ac12c15h16 111.5599

ac12c15h18 110.2542
d1 122.5551
d2 0.001
d3 58.6513
d4 180.0002
d5 58.2567
d6 179.9996
d7 60.5004
d8 180.0001
d9 179.9998
d10 179.9758

AA-1-hexyne, core-ionized state, C2*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.1575
rc6c2 1.4497
rc1h5 1.0764
rc6h7 1.0937
rc6c9 1.5448
rc9h10 1.0928
rc9c12 1.5349
rc12h13 1.0944
rc12c15 1.5311
rc15h16 1.0922
rc15h18 1.0912
ac2c6h7 106.5337
ac2c6c9 112.2225
ac6c9h10 109.1727
ac6c9c12 110.2278
ac9c12h13 109.4719
ac9c12c15 111.7223

ac12c15h16 111.5096
ac12c15h18 110.4261
d1 122.4138
d2 -0.0029
d3 58.6867
d4 179.9995
d5 58.2227
d6 180.0008
d7 60.418
d8 179.9998
d9 180.0005
d10 180.0725

AA-1-hexyne, core-ionized state, C3*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.1948
rc6c2 1.4083
rc1h5 1.0681
rc6h7 1.0402
rc6c9 1.5628
rc9h10 1.0891
rc9c12 1.5234
rc12h13 1.0948
rc12c15 1.5337
rc15h16 1.0916
rc15h18 1.0904
ac2c6h7 110.5506
ac2c6c9 114.6566
ac6c9h10 105.3813
ac6c9c12 110.9122
ac9c12h13 109.9026

ac9c12c15 110.4235
ac12c15h16 111.5572
ac12c15h18 109.9047
d1 121.6337
d2 0.0001
d3 57.4813
d4 180.0
d5 58.8865
d6 180.0
d7 60.6404
d8 180.0
d9 179.9997
d10 179.9956

AA-1-hexyne, core-ionized state, C4*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.2011
rc6c2 1.4522
rc1h5 1.0671
rc6h7 1.0917
rc6c9 1.5279
rc9h10 1.0348
rc9c12 1.5251
rc12h13 1.0899
rc12c15 1.5228
rc15h16 1.0918
rc15h18 1.0906
ac2c6h7 111.7306
ac2c6c9 111.0999
ac6c9h10 108.6732
ac6c9c12 114.405

ac9c12h13 106.4389
ac9c12c15 111.6582
ac12c15h16 112.0541
ac12c15h18 108.6678
d1 119.4572
d2 -0.0003
d3 57.3238
d4 180.0
d5 57.5899
d6 180.0
d7 61.3936
d8 180.0
d9 180.0019
d10 179.9958

AA-1-hexyne, core-ionized state, C5*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.2015
rc6c2 1.4573
rc1h5 1.0658
rc6h7 1.0962
rc6c9 1.5361
rc9h10 1.0891
rc9c12 1.5259
rc12h13 1.0347
rc12c15 1.5126
rc15h16 1.0876
rc15h18 1.0883
ac2c6h7 109.5488
ac2c6c9 110.123
ac6c9h10 111.2669

ac6c9c12 111.5693
ac9c12h13 108.8537
ac9c12c15 114.0407
ac12c15h16 108.8098
ac12c15h18 109.2769
d1 121.4375
d2 -0.0021
d3 60.495
d4 180.0004
d5 57.5643
d6 179.9999
d7 59.8662
d8 179.9999
d9 180.001
d10 180.1431

AA-1-hexyne, core-ionized state, C6*:

C
C 1 rc1c2
X 1 1.0 2 90.0
X 2 1.0 1 90.0 3 0.0
H 1 rc1h5 3 90.0 2 d9
C 2 rc6c2 4 90.0 1 d10
H 6 rc6h7 2 ac2c6h7 4 d1
H 6 rc6h7 2 ac2c6h7 4 -d1
C 6 rc6c9 2 ac2c6c9 4 d2
H 9 rc9h10 6 ac6c9h10 2 d3
H 9 rc9h10 6 ac6c9h10 2 -d3
C 9 rc9c12 6 ac6c9c12 2 d4
H 12 rc12h13 9 ac9c12h13 6 d5
H 12 rc12h13 9 ac9c12h13 6 -d5
C 12 rc12c15 9 ac9c12c15 6 d6
H 15 rc15h16 12 ac12c15h16 9 d7
H 15 rc15h16 12 ac12c15h16 9 -d7
H 15 rc15h18 12 ac12c15h18 9 d8
Variables:
rc1c2 1.2023
rc6c2 1.4585
rc1h5 1.0651
rc6h7 1.0952
rc6c9 1.5439
rc9h10 1.0938
rc9c12 1.5254
rc12h13 1.09
rc12c15 1.5371
rc15h16 1.0363
rc15h18 1.036
ac2c6h7 109.373
ac2c6c9 111.5984

ac6c9h10 108.9605
ac6c9c12 110.9284
ac9c12h13 112.2166
ac9c12c15 110.9638
ac12c15h16 110.7688
ac12c15h18 111.6312
d1 121.8302
d2 -0.0002
d3 58.3685
d4 180.0
d5 61.1715
d6 180.0
d7 59.6251
d8 180.0
d9 180.0001
d10 180.0016

AG-1-hexyne, ground state:

C
C,1,rc1c2
X,1,1.,2,90.
X,2,1.,1,90.,3,0.,0
H,1,rc1h5,3,90.,2,d9,0
C,2,rc6c2,4,90.,1,d10,0
H,6,rc6h7,2,ac2c6h7,4,d1,0
H,6,rc6h8,2,ac2c6h8,4,d12,0
C,6,rc6c9,2,ac2c6c9,4,d2,0
H,9,rc9h10,6,ac6c9h10,2,d3,0
H,9,rc9h11,6,ac6c9h11,2,d11,0
C,9,rc9c12,6,ac6c9c12,2,d4,0
H,12,rc12h13,9,ac9c12h13,6,d5,0
H,12,rc12h14,9,ac9c12h14,6,d13,0
C,12,rc12c15,9,ac9c12c15,6,d6,0
H,15,rc15h16,12,ac12c15h16,9,d7,0
H,15,rc15h17,12,ac12c15h17,9,d14,0
H,15,rc15h18,12,ac12c15h18,9,d8,0
Variables:
rc1c2 1.2047
rc6c2 1.4609
rc1h5 1.0632
rc6h7 1.0943
rc6h8 1.0955
rc6c9 1.5436
rc9h10 1.0936
rc9h11 1.0939
rc9c12 1.5348
rc12h13 1.0946
rc12h14 1.0954
rc12c15 1.5328

rc15h16	1.0927
rc15h17	1.0933
rc15h18	1.0928
ac2c6h7	108.6377
ac2c6h8	109.0489
ac2c6c9	113.0315
ac6c9h10	108.318
ac6c9h11	108.977
ac6c9c12	113.5222
ac9c12h13	108.2028
ac9c12h14	109.3651
ac9c12c15	114.4756
ac12c15h16	112.1506
ac12c15h17	111.1727
ac12c15h18	110.9757
d1	187.7098
d2	65.0471
d3	-55.9156
d4	182.3199
d5	172.097
d6	-66.2996
d7	63.4561
d8	183.2941
d9	180.1908
d10	180.8144
d11	59.3921
d12	-56.9262
d13	57.1362
d14	-57.0054

AG-1-hexyne, core-ionized state, C1*:

6	3.087432	-0.064631	-0.236513
6	1.973625	-0.216424	0.076064
1	4.071149	0.061570	-0.508132
6	0.602170	-0.357590	0.435065
1	0.284395	-1.357846	0.113827
1	0.548563	-0.330070	1.531462
6	-0.290941	0.760128	-0.207169
1	0.088557	1.733448	0.110156
1	-0.198307	0.701383	-1.293727
6	-1.757047	0.595128	0.218026
1	-2.292443	1.457509	-0.189041
1	-1.833871	0.678637	1.306289
6	-2.422072	-0.693815	-0.268499
1	-1.981105	-1.592038	0.174575
1	-2.368286	-0.789100	-1.355480
1	-3.477658	-0.700275	0.008232

AG-1-hexyne, core-ionized state, C2*:

6	3.089811	-0.066380	-0.236271
6	1.985400	-0.213871	0.077750
1	4.117680	0.067813	-0.526288
6	0.590936	-0.355089	0.441445
1	0.286981	-1.356997	0.127657
1	0.544264	-0.312073	1.533456
6	-0.285048	0.742169	-0.207896
1	0.097510	1.719735	0.095619
1	-0.194545	0.671189	-1.294772
6	-1.755053	0.597817	0.214845
1	-2.283883	1.463526	-0.192751
1	-1.833392	0.683820	1.302914
6	-2.435628	-0.685701	-0.268528
1	-2.008718	-1.586976	0.180978
1	-2.375033	-0.787503	-1.354669
1	-3.493371	-0.676205	-0.000218

AG-1-hexyne, core-ionized state, C3*:

6	3.109780	-0.118139	-0.221365
6	1.957120	-0.194664	0.083736
1	4.140813	-0.048078	-0.491261
6	0.598205	-0.287087	0.439311
1	0.212308	-1.220275	0.187190
1	0.482603	-0.200894	1.469327
6	-0.321496	0.786573	-0.228829
1	0.086291	1.747378	0.081552
1	-0.166498	0.665361	-1.300057
6	-1.774914	0.593210	0.183274
1	-2.323876	1.410811	-0.292028
1	-1.883735	0.751445	1.260840
6	-2.381630	-0.748710	-0.237914
1	-1.934146	-1.604872	0.280054
1	-2.292480	-0.913236	-1.314053
1	-3.443662	-0.774733	0.009151

AG-1-hexyne, core-ionized state, C4*:

6	3.136771	-0.036747	-0.255322
6	1.991843	-0.194303	0.072006
1	4.157551	0.094775	-0.537189
6	0.607095	-0.384071	0.467017
1	0.236923	-1.364745	0.167794
1	0.477373	-0.285906	1.546636
6	-0.290896	0.666001	-0.188545
1	0.089146	1.599580	0.044087
1	-0.206772	0.572435	-1.215688
6	-1.767316	0.610298	0.208186
1	-2.225552	1.504201	-0.216085

1	-1.798765	0.700005	1.294076
6	-2.465046	-0.649739	-0.283040
1	-2.076173	-1.556306	0.181741
1	-2.407337	-0.752780	-1.368647
1	-3.521097	-0.579900	-0.018537

AG-1-hexyne, core-ionized state, C5*:

6	3.136001	-0.023031	-0.253937
6	1.992300	-0.199097	0.069728
1	4.152622	0.133688	-0.532919
6	0.600665	-0.413751	0.446604
1	0.284854	-1.407263	0.114410
1	0.507283	-0.392646	1.538919
6	-0.276578	0.681060	-0.180064
1	0.071454	1.666236	0.129932
1	-0.252164	0.636474	-1.268098
6	-1.743041	0.576523	0.241931
1	-2.225259	1.441198	-0.056880
1	-1.791752	0.566301	1.275609
6	-2.496514	-0.615628	-0.306544
1	-2.043070	-1.529908	0.065316
1	-2.447725	-0.589818	-1.392843
1	-3.533239	-0.560721	0.020243

AG-1-hexyne, core-ionized state, C6*:

6	3.133215	-0.058888	-0.269450
6	1.992291	-0.193497	0.084166
1	4.148484	0.051725	-0.572565
6	0.599870	-0.338668	0.491649
1	0.281564	-1.365120	0.261385
1	0.524034	-0.228599	1.579194
6	-0.309648	0.699844	-0.199317
1	0.029216	1.701877	0.072800
1	-0.203766	0.634001	-1.285946
6	-1.777872	0.613774	0.201616
1	-2.362508	1.423768	-0.233310
1	-1.912114	0.633307	1.283286
6	-2.430154	-0.693381	-0.288382
1	-1.949000	-1.518588	0.112313
1	-2.373163	-0.766008	-1.320378
1	-3.428953	-0.741467	-0.018467

GA-1-hexyne, ground state:

C							
C	1	rc1c2					
X	1	1.	2	90.			
X	2	1.	1	90.	3	0.	0

```
H               1    rc1h5    3     90.      2    d9       0
C               2    rc6c2    4     90.      1    d10      0
H               6    rc6h7    2    ac2c6h7  4    d1       0
H               6    rc6h8    2    ac2c6h8  4    d12      0
C               6    rc6c9    2    ac2c6c9  4    d2       0
H               9    rc9h10   6    ac6c9h10 2    d3       0
H               9    rc9h11   6    ac6c9h11 2    d11      0
C               9    rc9c12   6    ac6c9c12 2    d4       0
H               12   rc12h13  9    ac9c12h13 6    d5       0
H               12   rc12h14  9    ac9c12h14 6    d13      0
C               12   rc12c15  9    ac9c12c15 6    d6       0
H               15   rc15h16  12   ac12c15h16 9    d7       0
H               15   rc15h17  12   ac12c15h17 9    d14      0
H               15   rc15h18  12   ac12c15h18 9    d8       0
```

Variables:

rc1c2	1.2048
rc6c2	1.4621
rc1h5	1.0632
rc6h7	1.095
rc6h8	1.0954
rc6c9	1.5434
rc9h10	1.094
rc9h11	1.095
rc9c12	1.5317
rc12h13	1.0938
rc12h14	1.0953
rc12c15	1.5312
rc15h16	1.0935
rc15h17	1.0932
rc15h18	1.0927
ac2c6h7	108.4893
ac2c6h8	108.9358
ac2c6c9	113.8504
ac6c9h10	108.9881
ac6c9h11	107.9246
ac6c9c12	113.8084
ac9c12h13	109.2551
ac9c12h14	109.2182
ac9c12c15	112.6672
ac12c15h16	111.4568
ac12c15h17	111.2196
ac12c15h18	111.3476
d1	136.0924
d2	13.9758
d3	57.1979
d4	-65.717
d5	57.2533
d6	179.4571
d7	59.4863
d8	179.634

d9	180.0409
d10	180.5043
d11	172.5123
d12	-108.6463
d13	-58.4077
d14	-60.4155

GA-1-hexyne, core-ionized state, C1*:

6	-2.585149	-0.986428	-0.131540
6	-1.863876	-0.083453	0.025483
1	-3.220831	-1.783677	-0.265370
6	-0.982568	1.027187	0.193972
1	-1.460386	1.877799	-0.311074
1	-0.955743	1.253609	1.268140
6	0.454451	0.757411	-0.364079
1	0.384571	0.515019	-1.426542
1	0.967306	1.719217	-0.293163
6	1.219456	-0.320932	0.406876
1	0.687363	-1.277764	0.344569
1	1.255400	-0.054923	1.467950
6	2.642948	-0.496609	-0.129775
1	3.215958	0.428989	-0.043800
1	2.642144	-0.795439	-1.180195
1	3.172644	-1.265892	0.433864

GA-1-hexyne, core-ionized state, C2*:

6	-2.574831	-0.987209	-0.126900
6	-1.861034	-0.087926	0.018421
1	-3.238482	-1.824086	-0.261083
6	-0.968940	1.044193	0.190160
1	-1.442130	1.885146	-0.324825
1	-0.954311	1.264355	1.261577
6	0.450617	0.767801	-0.351273
1	0.390903	0.545208	-1.419669
1	0.977728	1.721495	-0.262195
6	1.209594	-0.328254	0.402203
1	0.674565	-1.281333	0.322256
1	1.243251	-0.080629	1.467956
6	2.634706	-0.504471	-0.130921
1	3.213725	0.415296	-0.025080
1	2.636364	-0.781549	-1.187449
1	3.157714	-1.288702	0.418372

GA-1-hexyne, core-ionized state, C3*:

6	-2.625217	-0.963398	-0.127994
6	-1.854794	-0.063060	0.024613
1	-3.312047	-1.770282	-0.262398

6	-0.959897	1.012629	0.190264
1	-1.335639	1.863296	-0.274768
1	-0.866720	1.252399	1.198316
6	0.484673	0.762694	-0.364349
1	0.348968	0.499280	-1.412406
1	0.982846	1.730945	-0.300208
6	1.213953	-0.314595	0.424577
1	0.651655	-1.250307	0.379935
1	1.277559	-0.022678	1.477791
6	2.623933	-0.524729	-0.141711
1	3.223472	0.385891	-0.083691
1	2.593588	-0.848660	-1.183795
1	3.140413	-1.297124	0.428826

GA-1-hexyne, core-ionized state, C4*:

6	-2.568142	-1.020956	-0.110565
6	-1.834491	-0.078878	0.020120
1	-3.221736	-1.856020	-0.229545
6	-0.958492	1.070335	0.161400
1	-1.336477	1.924682	-0.404867
1	-0.856010	1.375265	1.204748
6	0.448597	0.768127	-0.357360
1	0.377223	0.440952	-1.336537
1	0.994927	1.645897	-0.379106
6	1.218424	-0.274154	0.453909
1	0.588087	-1.161636	0.481589
1	1.295328	0.122100	1.466348
6	2.584481	-0.557258	-0.154003
1	3.216899	0.332609	-0.181508
1	2.506280	-0.966705	-1.163231
1	3.093214	-1.300443	0.461102

GA-1-hexyne, core-ionized state, C5*:

6	-2.285835	-1.184866	-0.106198
6	-1.742206	-0.115329	-0.003169
1	-2.818569	-2.103552	-0.206557
6	-0.997418	1.133296	0.136972
1	-1.438377	1.916726	-0.485699
1	-1.053595	1.492837	1.169481
6	0.466813	0.956547	-0.298731
1	0.533192	0.764337	-1.368727
1	1.068153	1.833100	-0.060496
6	1.088913	-0.243454	0.396501
1	0.410061	-1.026722	0.289737
1	1.146189	-0.058852	1.412503
6	2.446029	-0.645683	-0.125538
1	3.134117	0.188588	-0.007369
1	2.354873	-0.904058	-1.177999

1	2.806182	-1.505465	0.436098

GA-1-hexyne, core-ionized state, C6*:

6	-2.488659	-1.074065	-0.116563
6	-1.807315	-0.089676	0.006391
1	-3.119877	-1.923752	-0.237366
6	-0.960506	1.090108	0.164038
1	-1.387937	1.926613	-0.395747
1	-0.948295	1.400224	1.213756
6	0.482127	0.858508	-0.337954
1	0.448606	0.614964	-1.403990
1	1.050486	1.786571	-0.225436
6	1.151400	-0.273112	0.435717
1	0.564595	-1.189900	0.382391
1	1.306841	-0.020379	1.484410
6	2.535851	-0.603086	-0.144027
1	3.159892	0.223330	-0.114236
1	2.455448	-0.901300	-1.133046
1	2.992845	-1.368434	0.383651

GG_{trans}-1-hexyne, ground state:

```
C
C              1    rc1c2
X              1    1.       2     90.
X              2    1.       1     90.      3     0.       0
H              1    rc1h5    3     90.      2     d9       0
C              2    rc6c2    4     90.      1     d10      0
H              6    rc6h7    2     ac2c6h7  4     d1       0
H              6    rc6h8    2     ac2c6h8  4     d12      0
C              6    rc6c9    2     ac2c6c9  4     d2       0
H              9    rc9h10   6     ac6c9h10 2     d3       0
H              9    rc9h11   6     ac6c9h11 2     d11      0
C              9    rc9c12   6     ac6c9c12 2     d4       0
H              12   rc12h13  9     ac9c12h13 6    d5       0
H              12   rc12h14  9     ac9c12h14 6    d13      0
C              12   rc12c15  9     ac9c12c15 6    d6       0
H              15   rc15h16  12    ac12c15h16 9   d7       0
H              15   rc15h17  12    ac12c15h17 9   d14      0
H              15   rc15h18  12    ac12c15h18 9   d8       0
 Variables:
 rc1c2        1.2049
 rc6c2        1.4618
 rc1h5        1.0632
 rc6h7        1.0949
 rc6h8        1.0943
 rc6c9        1.545
rc9h10        1.0938
rc9h11        1.095
```

rc9c12	1.5342
rc12h13	1.0946
rc12h14	1.0939
rc12c15	1.5325
rc15h16	1.0925
rc15h17	1.0937
rc15h18	1.0928
ac2c6h7	108.6329
ac2c6h8	108.9354
ac2c6c9	113.7932
ac6c9h10	108.3668
ac6c9h11	107.7167
ac6c9c12	114.9258
ac9c12h13	108.1114
ac9c12h14	109.2295
ac9c12c15	114.2421
ac12c15h16	111.9608
ac12c15h17	111.4083
ac12c15h18	110.8958
d1	164.3538
d2	42.7113
d3	61.132
d4	-61.4085
d5	174.7985
d6	-63.5369
d7	64.3836
d8	183.926
d9	180.1875
d10	180.5808
d11	176.2071
d12	-80.5826
d13	59.6252
d14	-56.3121

GG_{trans}-1-hexyne, core-ionized state, C1*:

6	2.502507	-0.832894	0.192555
6	1.683163	-0.090808	-0.179565
1	3.225828	-1.490046	0.512811
6	0.677118	0.829289	-0.600343
1	1.190191	1.779288	-0.801643
1	0.279897	0.460531	-1.554439
6	-0.460162	1.009279	0.463408
1	-0.011784	1.365542	1.393074
1	-1.074591	1.824092	0.073672
6	-1.312198	-0.241631	0.700648
1	-2.017807	0.007525	1.497595
1	-0.693424	-1.051658	1.103921
6	-2.089492	-0.726089	-0.526916
1	-1.440023	-1.076881	-1.334092

1	-2.728753	0.062923	-0.929584
1	-2.735147	-1.564186	-0.260041

GG_{trans}-1-hexyne, core-ionized state, C2*:

6	2.477593	-0.845035	0.184739
6	1.672645	-0.094181	-0.172411
1	3.226213	-1.544607	0.514824
6	0.665333	0.862215	-0.591753
1	1.190896	1.806522	-0.758641
1	0.285142	0.509988	-1.554089
6	-0.464417	1.020428	0.451569
1	-0.030073	1.392147	1.382959
1	-1.096756	1.821422	0.059111
6	-1.301567	-0.239543	0.700298
1	-2.016442	0.005276	1.490113
1	-0.674132	-1.035611	1.116953
6	-2.062388	-0.751161	-0.526761
1	-1.400350	-1.093601	-1.327228
1	-2.714031	0.021589	-0.940977
1	-2.693660	-1.599457	-0.257116

GG_{trans}-1-hexyne, core-ionized state, C3*:

6	2.529539	-0.784600	0.221871
6	1.656482	-0.071833	-0.174774
1	3.309432	-1.424104	0.573446
6	0.629392	0.776591	-0.631681
1	1.023768	1.691424	-0.928370
1	0.171047	0.368918	-1.473043
6	-0.505564	1.057862	0.411197
1	0.000299	1.466275	1.284768
1	-1.119206	1.833826	-0.048577
6	-1.306306	-0.198085	0.720597
1	-2.045686	0.105849	1.466695
1	-0.666758	-0.935176	1.212007
6	-2.013001	-0.807009	-0.493704
1	-1.314706	-1.217616	-1.231821
1	-2.661398	-0.083589	-0.994027
1	-2.640043	-1.643365	-0.182112

GG_{trans}-1-hexyne, core-ionized state, C4*:

6	2.517932	-0.850829	0.121660
6	1.672832	-0.052307	-0.180304
1	3.267697	-1.563007	0.385059
6	0.652048	0.913803	-0.543131
1	1.067890	1.921940	-0.608617
1	0.195031	0.678365	-1.504722
6	-0.469486	0.961534	0.497759

1	-0.051450	1.218084	1.408362
1	-1.122481	1.722245	0.243865
6	-1.267257	-0.335141	0.677162
1	-1.898813	-0.177441	1.551829
1	-0.537620	-1.107577	0.916134
6	-2.097760	-0.686702	-0.547711
1	-1.485146	-0.920874	-1.418806
1	-2.803351	0.105145	-0.808421
1	-2.681609	-1.579026	-0.317295

GG_{trans}-1-hexyne, core-ionized state, C5*:

6	2.302588	-0.966315	0.144833
6	1.587381	-0.055473	-0.185539
1	2.968569	-1.760943	0.395885
6	0.666819	1.028125	-0.516926
1	1.175381	1.994189	-0.453192
1	0.322067	0.933054	-1.550240
6	-0.517959	1.066381	0.465001
1	-0.177468	1.378680	1.451802
1	-1.300455	1.746129	0.130301
6	-1.132548	-0.316542	0.634201
1	-1.691215	-0.340698	1.503045
1	-0.331183	-0.970210	0.770219
6	-1.978461	-0.796849	-0.520413
1	-1.377309	-0.802367	-1.425740
1	-2.827861	-0.127806	-0.639006
1	-2.327440	-1.805995	-0.310012

GG_{trans}-1-hexyne, core-ionized state, C6*:

6	-2.158188	-0.814511	-0.300710
6	-1.456484	0.106992	0.034515
1	-2.834979	-1.577706	-0.612851
6	-0.544291	1.168724	0.458170
1	-1.006122	2.141962	0.272234
1	-0.423011	1.113558	1.545475
6	0.843946	1.132430	-0.238503
1	0.799419	1.682516	-1.180498
1	1.564570	1.659040	0.391393
6	1.364958	-0.260725	-0.595810
1	2.426621	-0.240031	-0.838298
1	0.821734	-0.681454	-1.440122
6	1.172497	-1.264170	0.547145
1	0.142478	-1.372808	0.698287
1	1.611321	-0.945772	1.428387
1	1.563342	-2.191733	0.307149

1-Pentene (*I*), ground state:

```
c
c   1 cc2
c   2 cc3       1 ccc3
c   3 cc4       2 ccc4       1 dih4
c   4 cc5       3 ccc5       2 dih5
h   1 hc6       2 hcc6       3 dih6
h   1 hc7       2 hcc7       3 dih7
h   2 hc8       3 hcc8       4 dih8
h   3 hc9       2 hcc9       1 dih9
h   3 hc10      2 hcc10      1 dih10
h   4 hc11      3 hcc11      2 dih11
h   4 hc12      3 hcc12      2 dih12
h   5 hc13      4 hcc13      3 dih13
h   5 hc14      4 hcc14      3 dih14
h   5 hc15      4 hcc15      3 dih15

      cc2       1.3314
      cc3       1.5019
     ccc3      125.3236
      cc4       1.5399
     ccc4      113.0025
     dih4      118.1173
      cc5       1.531
     ccc5      112.6895
     dih5      177.912
      hc6       1.0855
     hcc6      121.6857
     dih6        0.7701
      hc7       1.0843
     hcc7      121.6873
     dih7     -179.4638
      hc8       1.0889
     hcc8      115.9037
     dih8      -60.9526
      hc9       1.0972
     hcc9      109.1777
     dih9     -121.0379
     hc10       1.0944
     hcc10     109.7344
     dih10      -4.7103
     hc11       1.095
     hcc11     109.2396
     dih11      55.7393
     hc12       1.094
     hcc12     108.9928
     dih12     -59.7222
     hc13       1.0933
     hcc13     111.3109
     dih13     -60.1013
     hc14       1.0928
```

hcc14 111.3612
dih14 179.7645
hc15 1.0933
hcc15 111.2595
dih15 59.7242

1-Pentene (*I*), core-ionized state, C1*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
```

Variables:

cc2 1.3096
cc3 1.462
ccc3 125.1971
cc4 1.57
ccc4 109.848
dih4 114.433
cc5 1.5303
ccc5 110.4052
dih5 177.6946
hc6 1.0303
hcc6 121.7429
dih6 2.6704
hc7 1.0299
hcc7 121.9107
dih7 -177.7438
hc8 1.0885
hcc8 118.397
dih8 -63.2182
hc9 1.0971
hcc9 107.6012
dih9 -128.9778
hc10 1.091
hcc10 112.0457
dih10 -9.335
hc11 1.0927
hcc11 109.3174

dih11 56.1595
hc12 1.0921
hcc12 109.0133
dih12 -60.8177
hc13 1.0915
hcc13 111.5479
dih13 -61.1451
hc14 1.0914
hcc14 109.5153
dih14 179.4948
hc15 1.0915
hcc15 111.6699
dih15 60.2439

1-Pentene (*I*), core-ionized state, C2*:

c
c 1 cc2
c 2 cc3 1 ccc3
c 3 cc4 2 ccc4 1 dih4
c 4 cc5 3 ccc5 2 dih5
h 1 hc6 2 hcc6 3 dih6
h 1 hc7 2 hcc7 3 dih7
h 2 hc8 3 hcc8 4 dih8
h 3 hc9 2 hcc9 1 dih9
h 3 hc10 2 hcc10 1 dih10
h 4 hc11 3 hcc11 2 dih11
h 4 hc12 3 hcc12 2 dih12
h 5 hc13 4 hcc13 3 dih13
h 5 hc14 4 hcc14 3 dih14
h 5 hc15 4 hcc15 3 dih15

Variables:
cc2 1.2912
cc3 1.4881
ccc3 126.4797
cc4 1.5377
ccc4 111.6552
dih4 116.8498
cc5 1.5312
ccc5 110.6996
dih5 178.5315
hc6 1.0855
hcc6 120.1572
dih6 1.358
hc7 1.0853
hcc7 120.3792
dih7 -178.6943
hc8 1.0326
hcc8 115.2704
dih8 -61.6455

hc9 1.093
hcc9 106.9135
dih9 -122.1094
hc10 1.0904
hcc10 107.802
dih10 -6.1556
hc11 1.0942
hcc11 109.5434
dih11 57.1744
hc12 1.0932
hcc12 109.1789
dih12 -59.754
hc13 1.0917
hcc13 111.6661
dih13 -60.8599
hc14 1.0907
hcc14 109.9193
dih14 179.7216
hc15 1.092
hcc15 111.6296
dih15 60.3989

1-Pentene (*I*), core-ionized state, C3*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
```

Variables:
cc2 1.3218
cc3 1.4861
ccc3 122.0354
cc4 1.5382
ccc4 114.0598
dih4 117.6616
cc5 1.5211
ccc5 111.4835
dih5 180.0254
hc6 1.0845

hcc6 123.4829
dih6 0.4865
hc7 1.0826
hcc7 119.6095
dih7 -179.513
hc8 1.0814
hcc8 113.2694
dih8 -61.8653
hc9 1.0364
hcc9 109.8629
dih9 -120.5369
hc10 1.0345
hcc10 109.5793
dih10 -4.4637
hc11 1.0897
hcc11 106.1304
dih11 57.6302
hc12 1.089
hcc12 105.928
dih12 -57.2413
hc13 1.0919
hcc13 112.145
dih13 -61.8062
hc14 1.0908
hcc14 108.6135
dih14 179.6351
hc15 1.0919
hcc15 112.0961
dih15 61.1182

1-Pentene (*I*), core-ionized state, C4*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
 Variables:
 cc2       1.3301
 cc3       1.5003
```

ccc3	122.9786
cc4	1.5379
ccc4	111.3531
dih4	115.0542
cc5	1.5093
ccc5	114.378
dih5	179.04
hc6	1.0852
hcc6	122.38
dih6	-0.9512
hc7	1.0835
hcc7	121.0958
dih7	-182.2
hc8	1.0871
hcc8	116.7748
dih8	-67.7282
hc9	1.0915
hcc9	112.2656
dih9	-126.4035
hc10	1.0895
hcc10	111.9737
dih10	-4.1296
hc11	1.0343
hcc11	108.5308
dih11	56.1913
hc12	1.0344
hcc12	107.9804
dih12	-58.1085
hc13	1.0877
hcc13	108.9046
dih13	-60.1427
hc14	1.0883
hcc14	109.3626
dih14	179.7218
hc15	1.0877
hcc15	108.8863
dih15	59.6122

1-Pentene (*I*), core-ionized state, C5*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
```

h 4 hc11 3 hcc11 2 dih11
h 4 hc12 3 hcc12 2 dih12
h 5 hc13 4 hcc13 3 dih13
h 5 hc14 4 hcc14 3 dih14
h 5 hc15 4 hcc15 3 dih15

Variables:

cc2	1.3293
cc3	1.5082
ccc3	123.9357
cc4	1.5307
ccc4	110.2211
dih4	113.4398
cc5	1.5406
ccc5	111.3229
dih5	176.9935
hc6	1.085
hcc6	122.3185
dih6	0.3214
hc7	1.0834
hcc7	121.1565
dih7	-180.6369
hc8	1.0868
hcc8	116.2251
dih8	-67.2126
hc9	1.0968
hcc9	109.6798
dih9	-125.9033
hc10	1.0941
hcc10	109.8498
dih10	-7.9878
hc11	1.0897
hcc11	112.0403
dih11	58.0511
hc12	1.0892
hcc12	111.7374
dih12	-63.9255
hc13	1.036
hcc13	110.7384
dih13	-59.472
hc14	1.0357
hcc14	111.4935
dih14	180.1362
hc15	1.036
hcc15	110.711
dih15	59.8394

1-Pentene (*II*), ground state:

c
c 1 cc2

```
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
 Variables:
 cc2        1.3312
 cc3        1.5027
ccc3       125.6089
 cc4        1.5422
ccc4       113.5674
dih4      -121.5401
 cc5        1.5309
ccc5       113.6607
dih5        67.0241
 hc6        1.0855
hcc6       121.7035
dih6        0.1899
 hc7        1.0842
hcc7       121.677
dih7       180.4092
 hc8        1.0893
hcc8       115.6706
dih8        58.4692
 hc9        1.097
hcc9       108.5733
dih9       117.9592
hc10        1.0946
hcc10      109.7153
dih10       1.8057
hc11        1.0952
hcc11      109.0936
dih11      -55.7444
hc12        1.0944
hcc12      108.5293
dih12     -170.9119
hc13        1.0922
hcc13      111.501
dih13      -59.6993
hc14        1.0929
hcc14      111.1203
dih14      179.9637
```

hc15 1.0933
hcc15 111.1396
dih15 60.1087

1-Pentene (*II*), core-ionized state, C1*:

c
c 1 cc2
c 2 cc3 1 ccc3
c 3 cc4 2 ccc4 1 dih4
c 4 cc5 3 ccc5 2 dih5
h 1 hc6 2 hcc6 3 dih6
h 1 hc7 2 hcc7 3 dih7
h 2 hc8 3 hcc8 4 dih8
h 3 hc9 2 hcc9 1 dih9
h 3 hc10 2 hcc10 1 dih10
h 4 hc11 3 hcc11 2 dih11
h 4 hc12 3 hcc12 2 dih12
h 5 hc13 4 hcc13 3 dih13
h 5 hc14 4 hcc14 3 dih14
h 5 hc15 4 hcc15 3 dih15

Variables:
cc2 1.3089
cc3 1.4635
ccc3 125.4267
cc4 1.5661
ccc4 111.2891
dih4 -120.0422
cc5 1.528
ccc5 113.504
dih5 68.3177
hc6 1.0304
hcc6 121.7258
dih6 -0.9876
hc7 1.03
hcc7 121.919
dih7 179.3786
hc8 1.0888
hcc8 118.1756
dih8 58.8811
hc9 1.0994
hcc9 106.1565
dih9 123.4731
hc10 1.0912
hcc10 111.8736
dih10 5.0912
hc11 1.0928
hcc11 109.3027
dih11 -56.3215
hc12 1.0914

hcc12 105.6193
dih12 -170.5054
hc13 1.0937
hcc13 112.5822
dih13 -65.2985
hc14 1.0913
hcc14 109.8454
dih14 175.5323
hc15 1.0923
hcc15 111.7127
dih15 56.6271

1-Pentene (*II*), core-ionized state, C2*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
```

Variables:

cc2 1.291
cc3 1.4886
ccc3 126.4813
cc4 1.5391
ccc4 111.8549
dih4 -114.4898
cc5 1.5287
ccc5 114.0679
dih5 65.2988
hc6 1.0853
hcc6 120.1809
dih6 -1.5662
hc7 1.0853
hcc7 120.3517
dih7 178.5967
hc8 1.0326
hcc8 115.266
dih8 63.8371
hc9 1.0926
hcc9 106.6944

dih9 124.3471
hc10 1.0903
hcc10 107.6161
dih10 8.3124
hc11 1.094
hcc11 109.6
dih11 -59.8117
hc12 1.0927
hcc12 105.6967
dih12 -173.5506
hc13 1.0932
hcc13 112.683
dih13 -64.3174
hc14 1.0911
hcc14 110.0034
dih14 176.7231
hc15 1.0926
hcc15 111.6233
dih15 57.787

1-Pentene (*II*), core-ionized state, C3*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
h              5   hc13    4   hcc13   3   dih13
h              5   hc14    4   hcc14   3   dih14
h              5   hc15    4   hcc15   3   dih15
```

Variables:
cc2 1.3217
cc3 1.4863
ccc3 122.2364
cc4 1.5425
ccc4 114.7086
dih4 -120.4443
cc5 1.519
ccc5 112.2052
dih5 67.0749
hc6 1.0844
hcc6 123.4752
dih6 0.1785

hc7	1.0826
hcc7	119.6155
dih7	180.2558
hc8	1.0817
hcc8	113.163
dih8	59.7768
hc9	1.036
hcc9	109.2593
dih9	117.9151
hc10	1.0346
hcc10	109.4244
dih10	1.9416
hc11	1.0898
hcc11	106.0097
dih11	-55.7823
hc12	1.0904
hcc12	105.9352
dih12	-170.6372
hc13	1.09
hcc13	112.2208
dih13	-61.8019
hc14	1.091
hcc14	108.2669
dih14	179.3984
hc15	1.092
hcc15	111.9818
dih15	61.1686

1-Pentene (*II*), core-ionized state, C4*:

c									
c		1	cc2						
c		2	cc3	1	ccc3				
c		3	cc4	2	ccc4	1	dih4		
c		4	cc5	3	ccc5	2	dih5		
h		1	hc6	2	hcc6	3	dih6		
h		1	hc7	2	hcc7	3	dih7		
h		2	hc8	3	hcc8	4	dih8		
h		3	hc9	2	hcc9	1	dih9		
h		3	hc10	2	hcc10	1	dih10		
h		4	hc11	3	hcc11	2	dih11		
h		4	hc12	3	hcc12	2	dih12		
h		5	hc13	4	hcc13	3	dih13		
h		5	hc14	4	hcc14	3	dih14		
h		5	hc15	4	hcc15	3	dih15		

Variables:

cc2	1.3299
cc3	1.499
ccc3	123.1985
cc4	1.5417

ccc4	112.0383
dih4	-118.9125
cc5	1.5104
ccc5	114.5704
dih5	67.0273
hc6	1.0851
hcc6	122.3456
dih6	2.13
hc7	1.0834
hcc7	121.0924
dih7	183.5071
hc8	1.0875
hcc8	116.5862
dih8	65.0943
hc9	1.0923
hcc9	111.4952
dih9	122.7316
hc10	1.0896
hcc10	112.0776
dih10	0.8841
hc11	1.0343
hcc11	108.4163
dih11	-55.3809
hc12	1.0338
hcc12	108.5505
dih12	-170.3468
hc13	1.0868
hcc13	108.7122
dih13	-57.8694
hc14	1.0884
hcc14	109.1844
dih14	181.7638
hc15	1.0877
hcc15	108.7665
dih15	61.791

1-Pentene (*II*), core-ionized state, C5*:

```
c
c              1   cc2
c              2   cc3     1   ccc3
c              3   cc4     2   ccc4    1   dih4
c              4   cc5     3   ccc5    2   dih5
h              1   hc6     2   hcc6    3   dih6
h              1   hc7     2   hcc7    3   dih7
h              2   hc8     3   hcc8    4   dih8
h              3   hc9     2   hcc9    1   dih9
h              3   hc10    2   hcc10   1   dih10
h              4   hc11    3   hcc11   2   dih11
h              4   hc12    3   hcc12   2   dih12
```

h	5	hc13	4	hcc13	3	dih13
h	5	hc14	4	hcc14	3	dih14
h	5	hc15	4	hcc15	3	dih15

Variables:

cc2	1.3335
cc3	1.5065
ccc3	124.3542
cc4	1.5343
ccc4	111.5232
dih4	-110.6457
cc5	1.5332
ccc5	109.6435
dih5	58.6437
hc6	1.0862
hcc6	122.234
dih6	-3.0854
hc7	1.0839
hcc7	121.3427
dih7	180.2649
hc8	1.0879
hcc8	116.3094
dih8	69.2894
hc9	1.0937
hcc9	110.6481
dih9	130.8186
hc10	1.0938
hcc10	110.9391
dih10	12.6181
hc11	1.0896
hcc11	111.5415
dih11	-58.935
hc12	1.089
hcc12	112.743
dih12	-181.5691
hc13	1.0444
hcc13	107.7587
dih13	-44.1727
hc14	1.0347
hcc14	112.5369
dih14	195.3619
hc15	1.035
hcc15	111.3998
dih15	73.5131

1-Pentene (*III*), ground state:

6	-2.319039	-0.232670	-0.276560
6	-1.124156	-0.376067	0.263397
6	-0.120397	0.732648	0.442190
6	1.160115	0.560116	-0.390898

6	2.003217	-0.657008	-0.007959
1	-2.671162	0.720745	-0.633340
1	-2.995373	-1.062590	-0.381545
1	-0.827692	-1.353870	0.608949
1	0.152810	0.800801	1.494372
1	-0.587190	1.677578	0.179993
1	1.763981	1.456650	-0.274508
1	0.892589	0.501389	-1.442637
1	2.275738	-0.629523	1.043748
1	2.921819	-0.685573	-0.585619
1	1.476047	-1.587725	-0.190430

1-Pentene (*III*), core-ionized state, C1*:

```
c
c  1 cc2
c  2 cc3      1 ccc3
c  3 cc4      2 ccc4      1 dih4
c  4 cc5      3 ccc5      2 dih5
h  1 hc6      2 hcc6      3 dih6
h  1 hc7      2 hcc7      3 dih7
h  2 hc8      3 hcc8      4 dih8
h  3 hc9      2 hcc9      1 dih9
h  3 hc10     2 hcc10     1 dih10
h  4 hc11     3 hcc11     2 dih11
h  4 hc12     3 hcc12     2 dih12
h  5 hc13     4 hcc13     3 dih13
h  5 hc14     4 hcc14     3 dih14
h  5 hc15     4 hcc15     3 dih15

   cc2       1.3091
   cc3       1.4633
  ccc3     125.0782
   cc4       1.5691
  ccc4     111.8791
  dih4    -121.6184
   cc5       1.5282
  ccc5     114.7263
  dih5     -64.9156
   hc6       1.0305
  hcc6     121.7557
  dih6      -1.2907
   hc7       1.0299
  hcc7     121.9327
  dih7     179.0702
   hc8       1.0878
  hcc8     118.5702
  dih8      57.386
   hc9       1.0994
  hcc9     106.5019
```

dih9 121.616
hc10 1.0913
hcc10 111.4053
dih10 3.519
hc11 1.0918
hcc11 104.8401
dih11 174.2876
hc12 1.0919
hcc12 109.0482
dih12 60.5686
hc13 1.0921
hcc13 111.7218
dih13 -55.5836
hc14 1.0913
hcc14 109.532
dih14 -174.3388
hc15 1.0929
hcc15 113.1584
dih15 66.8997

1-Pentene (*III*), core-ionized state, C2*:

```
c
c  1 cc2
c  2 cc3      1 ccc3
c  3 cc4      2 ccc4      1 dih4
c  4 cc5      3 ccc5      2 dih5
h  1 hc6      2 hcc6      3 dih6
h  1 hc7      2 hcc7      3 dih7
h  2 hc8      3 hcc8      4 dih8
h  3 hc9      2 hcc9      1 dih9
h  3 hc10     2 hcc10     1 dih10
h  4 hc11     3 hcc11     2 dih11
h  4 hc12     3 hcc12     2 dih12
h  5 hc13     4 hcc13     3 dih13
h  5 hc14     4 hcc14     3 dih14
h  5 hc15     4 hcc15     3 dih15

 cc2       1.2907
 cc3       1.4893
ccc3      126.4986
 cc4       1.5379
ccc4      112.0331
dih4     -120.2325
 cc5       1.5304
ccc5      114.2542
dih5      -62.624
 hc6       1.0856
hcc6      120.1889
dih6       -0.8814
```

hc7	1.0853
hcc7	120.3725
dih7	179.1863
hc8	1.0326
hcc8	115.0891
dih8	58.7572
hc9	1.0933
hcc9	106.6003
dih9	118.9008
hc10	1.0902
hcc10	107.5698
dih10	2.9999
hc11	1.0927
hcc11	105.6997
dih11	176.5668
hc12	1.093
hcc12	109.3213
dih12	62.4002
hc13	1.0924
hcc13	111.7376
dih13	-56.0951
hc14	1.0909
hcc14	110.0358
dih14	-175.191
hc15	1.0945
hcc15	112.9289
dih15	66.3498

1-Pentene (*III*), core-ionized state, C3*:

```
c
c   1 cc2
c   2 cc3       1 ccc3
c   3 cc4       2 ccc4       1 dih4
c   4 cc5       3 ccc5       2 dih5
h   1 hc6       2 hcc6       3 dih6
h   1 hc7       2 hcc7       3 dih7
h   2 hc8       3 hcc8       4 dih8
h   3 hc9       2 hcc9       1 dih9
h   3 hc10      2 hcc10      1 dih10
h   4 hc11      3 hcc11      2 dih11
h   4 hc12      3 hcc12      2 dih12
h   5 hc13      4 hcc13      3 dih13
h   5 hc14      4 hcc14      3 dih14
h   5 hc15      4 hcc15      3 dih15

     cc2        1.3221
     cc3        1.4865
    ccc3       121.734
     cc4        1.5434
```

ccc4	115.2266
dih4	-112.9001
cc5	1.5202
ccc5	112.4802
dih5	-66.7045
hc6	1.0847
hcc6	123.4986
dih6	-0.3427
hc7	1.0825
hcc7	119.6242
dih7	179.6659
hc8	1.08
hcc8	113.751
dih8	67.109
hc9	1.0363
hcc9	109.5271
dih9	124.9231
hc10	1.0341
hcc10	108.9566
dih10	9.1953
hc11	1.0906
hcc11	105.7428
dih11	171.4881
hc12	1.089
hcc12	105.8908
dih12	56.319
hc13	1.0921
hcc13	112.0931
dih13	-58.9218
hc14	1.091
hcc14	108.1682
dih14	-177.0539
hc15	1.0904
hcc15	112.5613
dih15	64.592

1-Pentene (*III*), core-ionized state, C4*:

```
c
c  1 cc2
c  2 cc3      1 ccc3
c  3 cc4      2 ccc4      1 dih4
c  4 cc5      3 ccc5      2 dih5
h  1 hc6      2 hcc6      3 dih6
h  1 hc7      2 hcc7      3 dih7
h  2 hc8      3 hcc8      4 dih8
h  3 hc9      2 hcc9      1 dih9
h  3 hc10     2 hcc10     1 dih10
h  4 hc11     3 hcc11     2 dih11
h  4 hc12     3 hcc12     2 dih12
```

```
h   5 hc13      4 hcc13      3 dih13
h   5 hc14      4 hcc14      3 dih14
h   5 hc15      4 hcc15      3 dih15

   cc2        1.3307
   cc3        1.5001
  ccc3      122.5907
   cc4        1.5427
  ccc4      112.4033
  dih4     -112.4629
   cc5        1.5104
  ccc5      115.0738
  dih5      -66.2181
   hc6        1.0853
  hcc6      122.4372
  dih6        1.333
   hc7        1.0835
  hcc7      121.0734
  dih7      182.562
   hc8        1.0854
  hcc8      117.3448
  dih8       71.2051
   hc9        1.0914
  hcc9      112.3103
  dih9      128.3609
  hc10        1.0901
  hcc10     111.2048
  dih10       6.5817
  hc11        1.0338
  hcc11     108.3669
  dih11     171.2813
  hc12        1.0344
  hcc12     107.9689
  dih12      56.267
  hc13        1.0878
  hcc13     108.852
  dih13     -57.9623
  hc14        1.0884
  hcc14     109.1277
  dih14    -177.906
  hc15        1.0866
  hcc15     109.1028
  dih15      62.2138
```

1-Pentene (*III*), core-ionized state, C5*:

```
c
c   1 cc2
c   2 cc3       1 ccc3
c   3 cc4       2 ccc4       1 dih4
```

```
c   4 cc5       3 ccc5       2 dih5
h   1 hc6       2 hcc6       3 dih6
h   1 hc7       2 hcc7       3 dih7
h   2 hc8       3 hcc8       4 dih8
h   3 hc9       2 hcc9       1 dih9
h   3 hc10      2 hcc10      1 dih10
h   4 hc11      3 hcc11      2 dih11
h   4 hc12      3 hcc12      2 dih12
h   5 hc13      4 hcc13      3 dih13
h   5 hc14      4 hcc14      3 dih14
h   5 hc15      4 hcc15      3 dih15

   cc2        1.3337
   cc3        1.512
  ccc3       126.5726
   cc4        1.5267
  ccc4       114.9669
  dih4       -25.0
   cc5        1.5337
  ccc5       109.916
  dih5       -57.1602
   hc6        1.0869
  hcc6       123.6162
  dih6        -2.1853
   hc7        1.0832
  hcc7       120.8135
  dih7       181.3989
   hc8        1.0858
  hcc8       114.798
  dih8       156.1328
   hc9        1.0946
  hcc9       109.5698
  dih9       210.8995
  hc10        1.0953
  hcc10      109.8007
  dih10       95.9068
  hc11        1.0889
  hcc11      112.0459
  dih11      183.4782
  hc12        1.0887
  hcc12      112.3485
  dih12       61.1351
  hc13        1.0352
  hcc13      111.3471
  dih13      -67.8284
  hc14        1.0348
  hcc14      112.4929
  dih14     -189.5822
  hc15        1.0431
  hcc15      107.6657
```

dih15 50.118

1-Pentene (*III*), core-ionized state, frozen dihedral C1-C2-C3-C4, C5*:

```
c
c   1 cc2
c   2 cc3       1 ccc3
c   3 cc4       2 ccc4       1 -120.
c   4 cc5       3 ccc5       2 dih5
h   1 hc6       2 hcc6       3 dih6
h   1 hc7       2 hcc7       3 dih7
h   2 hc8       3 hcc8       4 dih8
h   3 hc9       2 hcc9       1 dih9
h   3 hc10      2 hcc10      1 dih10
h   4 hc11      3 hcc11      2 dih11
h   4 hc12      3 hcc12      2 dih12
h   5 hc13      4 hcc13      3 dih13
h   5 hc14      4 hcc14      3 dih14
h   5 hc15      4 hcc15      3 dih15

 cc2        1.3303
 cc3        1.5073
ccc3       124.3634
 cc4        1.532
ccc4       114.3911
 cc5        1.5368
ccc5       111.5847
dih5       -56.9817
 hc6        1.0849
hcc6       122.024
dih6        2.5056
 hc7        1.0835
hcc7       121.3945
dih7       183.0094
 hc8        1.0906
hcc8       117.4516
dih8        65.7827
 hc9        1.0966
hcc9       110.2806
dih9       116.5558
hc10        1.0922
hcc10      110.1333
dih10       -0.2832
hc11        1.0896
hcc11      111.984
dih11      183.6914
hc12        1.0895
hcc12      111.5797
dih12       61.3935
hc13        1.0359
```

hcc13	111.1242
dih13	-60.1165
hc14	1.0355
hcc14	111.4129
dih14	-180.7542
hc15	1.0368
hcc15	110.0295
dih15	59.3231

1-Pentene (*IV*), ground state:

6	2.036729	-0.700212	0.004471
6	1.512223	0.529971	0.002543
6	0.044779	0.829659	-0.006442
6	-0.808920	-0.440757	-0.013319
6	-2.303218	-0.139857	0.010094
1	1.406472	-1.584807	-0.021239
1	3.108711	-0.865428	0.027968
1	2.180821	1.391505	0.007776
1	-0.204135	1.443190	-0.883220
1	-0.216740	1.408560	0.888060
1	-0.542502	-1.059590	0.852065
1	-0.558662	-1.028959	-0.903402
1	-2.573268	0.425105	0.907318
1	-2.896016	-1.058714	0.000503
1	-2.594236	0.456318	-0.859905

1-Pentene (*IV*), core-ionized state, C1*:

6	-2.089577	-0.655431	-0.000105
6	-1.513472	0.518195	-0.000054
6	-0.063494	0.742337	0.000140
6	0.854186	-0.482903	0.000272
6	2.333260	-0.082168	-0.000211
1	-1.534785	-1.524078	0.000003
1	-3.113895	-0.761545	-0.000253
1	-2.172338	1.384767	-0.000175
1	0.131422	1.406332	0.858665
1	0.131582	1.406200	-0.858451
1	0.645393	-1.096909	-0.882013
1	0.645812	-1.096453	0.882973
1	2.587313	0.505774	-0.884410
1	2.966201	-0.970063	-0.000405
1	2.587881	0.505789	0.883815

1-Pentene (*IV*), core-ionized state, C2*:

6	-2.096675	-0.643240	-0.000116
6	-1.507781	0.505735	-0.000106
6	-0.037231	0.768263	0.000221

6	0.838057	-0.479435	0.000320
6	2.323366	-0.097213	-0.000271
1	-1.514828	-1.557731	0.000185
1	-3.180384	-0.698168	-0.000414
1	-2.098991	1.351847	-0.000344
1	0.159845	1.391316	0.877605
1	0.160177	1.391290	-0.877106
1	0.619673	-1.089127	-0.882263
1	0.620192	-1.088698	0.883327
1	2.587283	0.485607	-0.884726
1	2.940456	-0.995954	-0.000897
1	2.588159	0.484967	0.884342

1-Pentene (*IV*), core-ionized state, C3*:

6	-2.100938	-0.653199	-0.000159
6	-1.524500	0.535064	-0.000069
6	-0.044459	0.747432	0.000182
6	0.857746	-0.486027	0.000391
6	2.327539	-0.087744	-0.000286
1	-1.565841	-1.593507	-0.000003
1	-3.182362	-0.705739	-0.000375
1	-2.072126	1.468362	-0.000171
1	0.204574	1.323322	0.825207
1	0.204823	1.323121	-0.824908
1	0.593837	-1.063925	-0.883844
1	0.594414	-1.063259	0.885233
1	2.597647	0.486356	-0.889057
1	2.934203	-0.994037	-0.000670
1	2.598504	0.486154	0.888232

1-Pentene (*IV*), core-ionized state, C4*:

6	-2.079684	-0.683824	-0.000066
6	-1.505919	0.514607	-0.000021
6	-0.035636	0.819684	0.000042
6	0.831544	-0.425751	0.000196
6	2.317597	-0.151210	-0.000129
1	-1.538051	-1.625577	-0.000056
1	-3.158270	-0.776965	-0.000124
1	-2.122594	1.407806	-0.000038
1	0.245890	1.403812	0.879052
1	0.245965	1.403612	-0.879076
1	0.581426	-0.997992	-0.825532
1	0.581699	-0.997629	0.826258
1	2.570110	0.419373	-0.890941
1	2.855926	-1.096927	-0.000203
1	2.570489	0.419450	0.890526

1-Pentene (*IV*), core-ionized state, C5*:

6	-2.103049	-0.664932	-0.000137
6	-1.507910	0.523701	-0.000095
6	-0.023704	0.796123	0.000192
6	0.825379	-0.469796	0.000389
6	2.321983	-0.122376	-0.000304
1	-1.569876	-1.609893	0.000076
1	-3.183431	-0.738731	-0.000372
1	-2.117808	1.421783	-0.000269
1	0.221748	1.407564	0.877416
1	0.222021	1.407439	-0.877043
1	0.649583	-1.080887	-0.883930
1	0.650261	-1.080250	0.885282
1	2.570739	0.436309	-0.836662
1	2.909009	-0.975892	-0.000627
1	2.571561	0.436236	0.835858

Trans-2-hexene (*I*), ground state:

6	-1.800470	-0.351456	-0.236185
6	-0.744394	0.079983	0.453347
6	0.643810	-0.487410	0.363010
6	1.679144	0.524797	-0.160922
6	3.100652	-0.042858	-0.193249
1	-1.669781	-1.191167	-0.917798
1	-0.873511	0.922657	1.132559
1	0.964010	-0.829335	1.355294
1	0.639220	-1.372888	-0.281143
1	1.655195	1.422028	0.466665
1	1.383113	0.849309	-1.163085
1	3.430232	-0.344275	0.804773
1	3.815741	0.692725	-0.570072
1	3.161676	-0.923751	-0.838267
6	-3.185444	0.221968	-0.154741
1	-3.234103	1.056006	0.548450
1	-3.522948	0.582546	-1.131809
1	-3.908637	-0.533997	0.166878

Trans-2-hexene (*I*), core-ionized state, C1*:

6	1.784965	0.391924	-0.247064
6	0.747209	-0.081209	0.432442
6	-0.630915	0.490297	0.363919
6	-1.660199	-0.529332	-0.172121
6	-3.078978	0.043836	-0.179570
1	1.765747	1.244619	-0.910894
1	0.876201	-0.952238	1.074744
1	-0.923612	0.788997	1.377103
1	-0.638543	1.395325	-0.248696
1	-1.629878	-1.433688	0.443986

1	-1.373343	-0.832239	-1.183131
1	-3.402245	0.321259	0.826240
1	-3.788116	-0.690666	-0.565013
1	-3.147730	0.932999	-0.810443
6	3.140754	-0.242324	-0.141864
1	3.117911	-1.052865	0.503120
1	3.477404	-0.585022	-1.062236
1	3.849184	0.424371	0.220773

Trans-2-hexene (*I*), core-ionized state, C2*:

6	-1.760170	-0.293936	-0.288317
6	-0.728125	-0.049504	0.472739
6	0.622656	-0.591209	0.270050
6	1.626015	0.559239	-0.065667
6	3.049688	0.015598	-0.205053
1	-1.633268	-0.943979	-1.078052
1	-0.888881	0.637746	1.301662
1	0.940629	-1.048516	1.214896
1	0.638579	-1.358525	-0.506481
1	1.587385	1.314967	0.723300
1	1.313218	1.046497	-0.992108
1	3.396386	-0.440726	0.724129
1	3.733212	0.829183	-0.453228
1	3.119554	-0.730725	-0.998733
6	-3.117337	0.270993	-0.127686
1	-3.140269	0.934137	0.734429
1	-3.388663	0.830179	-1.023359
1	-3.834245	-0.537328	0.017145

Trans-2-hexene (*I*), core-ionized state, C3*:

6	-1.774526	-0.329953	-0.253329
6	-0.741905	0.032922	0.450515
6	0.636908	-0.515905	0.339145
6	1.643171	0.547802	-0.122161
6	3.057564	-0.032250	-0.200105
1	-1.613493	-1.123640	-0.980475
1	-0.865332	0.785921	1.144151
1	0.912167	-0.906099	1.321763
1	0.604217	-1.357575	-0.353940
1	1.626212	1.392845	0.573056
1	1.336297	0.933351	-1.098338
1	3.398805	-0.391565	0.772989
1	3.759371	0.732793	-0.534473
1	3.113229	-0.863142	-0.906803
6	-3.122874	0.246184	-0.135581
1	-3.200859	1.033341	0.612609
1	-3.429593	0.629953	-1.115977
1	-3.831046	-0.558983	0.094528

Trans-2-hexene (*I*), core-ionized state, C4*:

6	-1.767577	-0.394659	-0.145622
6	-0.745445	0.234726	0.422917
6	0.620795	-0.349802	0.445343
6	1.687220	0.502410	-0.256143
6	3.061308	-0.146420	-0.179568
1	-1.606351	-1.367690	-0.607762
1	-0.807540	1.200053	0.906805
1	0.922924	-0.505392	1.424124
1	0.600174	-1.284717	0.003432
1	1.666536	1.476209	0.232238
1	1.343353	0.630759	-1.281425
1	3.398233	-0.274578	0.851219
1	3.782742	0.500233	-0.680784
1	3.085738	-1.115311	-0.682675
6	-3.157499	0.143730	-0.201521
1	-3.245560	1.117606	0.279596
1	-3.484780	0.234065	-1.241187
1	-3.848277	-0.551149	0.283981

Trans-2-hexene (*I*), core-ionized state, C5*:

6	1.758293	0.289916	-0.284195
6	0.737453	-0.055007	0.505790
6	-0.630715	0.536221	0.373580
6	-1.657164	-0.510629	-0.111569
6	-3.066710	0.008276	-0.237554
1	1.583988	1.019383	-1.074727
1	0.893500	-0.754730	1.323793
1	-1.021003	0.908698	1.322425
1	-0.658684	1.347943	-0.352898
1	-1.633745	-1.312003	0.541114
1	-1.327307	-0.876664	-1.020389
1	-3.400596	0.361708	0.735430
1	-3.718455	-0.791452	-0.584364
1	-3.078091	0.829702	-0.950603
6	3.154945	-0.220496	-0.163333
1	3.261704	-0.950473	0.639468
1	3.478323	-0.679752	-1.102134
1	3.843747	0.607953	0.026567

Trans-2-hexene (*I*), core-ionized state, C6*:

6	-1.767081	-0.285794	-0.297221
6	-0.732793	0.003214	0.493652
6	0.651096	-0.563985	0.311224
6	1.627625	0.540345	-0.101693
6	3.070408	0.004838	-0.204693

1	-1.614322	-0.972180	-1.129416
1	-0.870849	0.673121	1.339380
1	0.994966	-1.021900	1.247245
1	0.634963	-1.350097	-0.450298
1	1.654901	1.353432	0.623283
1	1.379109	0.955237	-1.077523
1	3.378737	-0.386955	0.703223
1	3.734928	0.750887	-0.476877
1	3.129449	-0.751666	-0.909745
6	-3.156083	0.241306	-0.130294
1	-3.237812	0.921990	0.718007
1	-3.481032	0.769360	-1.031749
1	-3.862071	-0.580768	0.018615

Trans-2-hexene (*II*), ground state:

6	-1.558095	-0.018710	0.406056
6	-0.549961	-0.549205	-0.285943
6	0.755063	-1.023414	0.290208
6	1.987153	-0.301907	-0.292419
6	2.063620	1.180108	0.083254
1	-1.448047	0.093420	1.483967
1	-0.659702	-0.658778	-1.365360
1	0.860553	-2.097391	0.093092
1	0.741797	-0.906863	1.379007
1	1.980341	-0.405952	-1.382745
1	2.889658	-0.813819	0.056264
1	1.182090	1.724461	-0.262413
1	2.944676	1.654532	-0.356169
1	2.123695	1.308905	1.167479
6	-2.861792	0.444964	-0.175651
1	-2.892583	0.301331	-1.257725
1	-3.706108	-0.097498	0.261401
1	-3.032296	1.506637	0.030177

Trans-2-hexene (*II*), core-ionized state, C1*:

6	-1.553430	-0.028757	0.444595
6	-0.558545	-0.518128	-0.285274
6	0.729497	-1.027306	0.277232
6	1.967451	-0.307052	-0.302457
6	2.071924	1.165059	0.100360
1	-1.557369	0.065259	1.521191
1	-0.658966	-0.563743	-1.369981
1	0.793972	-2.093105	0.028220
1	0.722388	-0.953822	1.367736
1	1.965787	-0.403428	-1.392704
1	2.850239	-0.847359	0.046958
1	1.231724	1.756562	-0.273422
1	2.984164	1.609263	-0.301974

1	2.103980	1.279660	1.186762
6	-2.824419	0.453984	-0.192156
1	-2.782175	0.349965	-1.222356
1	-3.648417	-0.082475	0.141778
1	-3.000192	1.456423	0.013986

Trans-2-hexene (*II*), core-ionized state, C2*:

6	-1.538910	-0.039558	0.392018
6	-0.540052	-0.533822	-0.286383
6	0.718034	-1.033285	0.289716
6	1.958246	-0.297750	-0.300128
6	2.042065	1.174220	0.104234
1	-1.448723	0.005096	1.417894
1	-0.656733	-0.566754	-1.368714
1	0.785080	-2.092125	0.001926
1	0.708438	-0.978503	1.380399
1	1.956935	-0.403146	-1.388335
1	2.834366	-0.840037	0.060023
1	1.207767	1.762914	-0.288477
1	2.959058	1.618921	-0.285744
1	2.059174	1.293245	1.190096
6	-2.810429	0.467063	-0.167823
1	-2.797659	0.375976	-1.251828
1	-3.642363	-0.110804	0.235280
1	-2.939063	1.514007	0.107674

Trans-2-hexene (*II*), core-ionized state, C3*:

6	-1.508376	-0.016159	0.394717
6	-0.545305	-0.584571	-0.270899
6	0.754072	-1.053614	0.284742
6	1.948164	-0.279309	-0.293358
6	1.970230	1.203067	0.081512
1	-1.351452	0.113777	1.463675
1	-0.667065	-0.717357	-1.286036
1	0.835606	-2.117948	0.053085
1	0.704455	-0.949775	1.369555
1	1.974917	-0.405257	-1.379956
1	2.844416	-0.775083	0.087631
1	1.114212	1.749647	-0.322924
1	2.866749	1.679625	-0.318044
1	1.983704	1.342749	1.165265
6	-2.776629	0.451304	-0.186688
1	-2.855093	0.288073	-1.260421
1	-3.605267	-0.049994	0.328122
1	-2.898113	1.517240	0.039881

Trans-2-hexene (*II*), core-ionized state, C4*:

6	-1.530985	-0.005743	0.398108
6	-0.553398	-0.554434	-0.313823
6	0.726514	-0.988028	0.305213
6	1.986512	-0.313410	-0.267206
6	2.041674	1.169081	0.059663
1	-1.395129	0.140466	1.468764
1	-0.597811	-0.740438	-1.378688
1	0.832019	-2.012473	0.196359
1	0.689803	-0.808752	1.323196
1	1.964954	-0.496879	-1.341133
1	2.836455	-0.851977	0.153447
1	1.198139	1.713762	-0.364449
1	2.955885	1.582506	-0.368542
1	2.074637	1.347781	1.136540
6	-2.837628	0.435561	-0.170052
1	-2.903486	0.264331	-1.244401
1	-3.657735	-0.096402	0.320256
1	-2.993855	1.499916	0.027235

Trans-2-hexene (*II*), core-ionized state, C5*:

6	-1.515419	0.035232	0.384951
6	-0.542791	-0.571089	-0.301147
6	0.739958	-1.021732	0.321266
6	1.967998	-0.292354	-0.274546
6	2.037367	1.179153	0.049683
1	-1.353344	0.252142	1.440267
1	-0.695589	-0.829327	-1.347161
1	0.923801	-2.084932	0.151182
1	0.764586	-0.834962	1.394660
1	1.949521	-0.417550	-1.300672
1	2.825407	-0.761796	0.060699
1	1.121791	1.652772	-0.294929
1	2.900307	1.617107	-0.448459
1	2.132412	1.296612	1.126938
6	-2.846919	0.423935	-0.165211
1	-2.943695	0.185509	-1.224815
1	-3.644432	-0.089602	0.380050
1	-3.021925	1.495162	-0.027734

Trans-2-hexene (*II*), core-ionized state, C6*:

6	-1.460775	-0.027751	0.390488
6	-0.474730	-0.601136	-0.309505
6	0.835108	-1.056626	0.278792
6	2.015774	-0.229380	-0.248095
6	1.773464	1.251295	0.063572
1	-1.326874	0.109637	1.464082
1	-0.617590	-0.786697	-1.373027
1	1.039539	-2.097556	0.012200

1	0.807290	-1.015096	1.371850
1	2.103033	-0.304778	-1.331575
1	2.967236	-0.511536	0.200511
1	0.767608	1.445356	-0.146880
1	2.371036	1.882578	-0.496932
1	1.928917	1.457657	1.065497
6	-2.788908	0.386695	-0.159342
1	-2.856204	0.228520	-1.236411
1	-3.587798	-0.186043	0.320849
1	-2.995792	1.439380	0.054365

1-Hexene (*II*), ground state:

6	3.086633	-0.177063	0.434170
6	2.041014	-0.202470	-0.389478
1	2.077752	-0.852920	-1.262110
1	3.969047	-0.780299	0.252673
1	3.099724	0.450255	1.320076
6	0.775757	0.587902	-0.215868
1	0.864558	1.239343	0.659157
1	0.643927	1.247674	-1.082821
6	-0.473521	-0.300957	-0.082620
1	-0.362092	-0.947057	0.794525
1	-0.533500	-0.973407	-0.946130
6	-1.774496	0.501876	0.028729
1	-1.877820	1.146762	-0.850548
1	-1.711082	1.175568	0.890134
6	-3.015420	-0.385167	0.163420
1	-2.955853	-1.018237	1.052790
1	-3.127370	-1.044629	-0.701382
1	-3.927090	0.212222	0.243523

1-Hexene (*II*), core-ionized state, C1*:

6	-2.973162	-0.345732	-0.410270
6	-2.005992	-0.054908	0.424843
1	-2.108762	-0.442920	1.436525
1	-3.785760	-0.910740	-0.126495
1	-2.963968	-0.015200	-1.385963
6	-0.794926	0.687715	0.085029
1	-0.861892	1.153667	-0.899189
1	-0.650888	1.467787	0.841742
6	0.441252	-0.278264	0.161498
1	0.309750	-1.087433	-0.561263
1	0.488840	-0.734738	1.153914
6	1.741760	0.486501	-0.127854
1	1.857206	1.290602	0.604752
1	1.671912	0.965014	-1.109171
6	2.959497	-0.440035	-0.086747
1	2.886431	-1.233003	-0.834252

1	3.075304	-0.908467	0.893080
1	3.871257	0.123773	-0.292672

1-Hexene (*II*), core-ionized state, C2*:

6	3.033309	-0.209742	0.421069
6	2.022619	-0.170054	-0.381185
1	2.054688	-0.749799	-1.235076
1	3.890175	-0.835379	0.192992
1	3.031951	0.383437	1.330160
6	0.769072	0.608576	-0.192494
1	0.886411	1.217363	0.704369
1	0.681793	1.281297	-1.049638
6	-0.458017	-0.312102	-0.101061
1	-0.339666	-0.990791	0.748898
1	-0.519877	-0.934024	-1.000300
6	-1.750141	0.503783	0.050997
1	-1.851276	1.185990	-0.798625
1	-1.680587	1.131286	0.945051
6	-2.987523	-0.392547	0.144951
1	-2.931391	-1.064736	1.004096
1	-3.108419	-1.003043	-0.752712
1	-3.889723	0.210917	0.257127

1-Hexene (*II*), core-ionized state, C3*:

6	3.024493	-0.124173	0.473799
6	2.037773	-0.229565	-0.399374
1	2.052037	-0.873849	-1.267775
1	3.923943	-0.711190	0.338867
1	2.989342	0.528735	1.339150
6	0.775469	0.541115	-0.261330
1	0.848304	1.187497	0.542951
1	0.635611	1.138639	-1.096388
6	-0.478323	-0.329652	-0.080351
1	-0.309992	-0.919739	0.820153
1	-0.503934	-1.009636	-0.932244
6	-1.743961	0.518984	0.010088
1	-1.849664	1.123117	-0.896916
1	-1.663083	1.215310	0.851155
6	-2.983112	-0.364681	0.189523
1	-2.923432	-0.958549	1.103617
1	-3.114860	-1.047033	-0.652538
1	-3.878299	0.254539	0.255837

1-Hexene (*II*), core-ionized state, C4*:

6	-3.005885	-0.310636	-0.436821
6	-2.028405	-0.117397	0.443988
1	-2.125761	-0.493142	1.459431

1	-3.905492	-0.850051	-0.165724
1	-2.958781	0.074783	-1.450178
6	-0.784503	0.661319	0.128378
1	-0.827401	1.107554	-0.864620
1	-0.601752	1.455386	0.854472
6	0.460083	-0.232957	0.155816
1	0.331096	-0.994116	-0.532197
1	0.522310	-0.694558	1.078967
6	1.769883	0.492060	-0.128866
1	1.857427	1.277987	0.620867
1	1.654867	0.967293	-1.102821
6	2.959409	-0.457888	-0.098224
1	2.879075	-1.238494	-0.857465
1	3.082924	-0.928146	0.879450
1	3.867993	0.108498	-0.305808

1-Hexene (*II*), core-ionized state, C5*:

6	-3.030770	-0.246202	-0.435829
6	-2.025159	-0.142553	0.427175
1	-2.090386	-0.636461	1.393398
1	-3.921069	-0.814354	-0.194322
1	-3.014589	0.240377	-1.405582
6	-0.763592	0.640197	0.164666
1	-0.856893	1.187570	-0.778177
1	-0.617946	1.381319	0.960513
6	0.446492	-0.297881	0.112426
1	0.371212	-1.001237	-0.716471
1	0.554226	-0.869427	1.034642
6	1.754591	0.471033	-0.077581
1	1.845801	1.158752	0.689690
1	1.686395	1.024981	-0.948367
6	2.987693	-0.399937	-0.127391
1	2.892285	-1.097235	-0.956575
1	3.068556	-0.948310	0.808355
1	3.866878	0.226089	-0.267890

1-Hexene (*II*), core-ionized state, C6*:

6	-3.048843	-0.210570	-0.442824
6	-2.029562	-0.174927	0.409878
1	-2.088144	-0.741501	1.336631
1	-3.939878	-0.790132	-0.232221
1	-3.041603	0.346224	-1.374268
6	-0.765326	0.613452	0.194483
1	-0.851017	1.208170	-0.719261
1	-0.628283	1.319205	1.022399
6	0.470829	-0.304350	0.107113
1	0.350207	-0.987376	-0.739948
1	0.531175	-0.920082	1.011068

6	1.749868	0.510181	-0.051975
1	1.926065	1.169491	0.797817
1	1.742394	1.113618	-0.959549
6	2.984102	-0.404834	-0.152424
1	2.901566	-1.041209	-0.965757
1	3.073560	-0.991551	0.696604
1	3.857549	0.141427	-0.259024

1-Butene (*AC*), ground state:

6	1.855088	0.013781	-0.284076
6	0.723312	-0.288557	0.348273
6	-0.539865	0.524446	0.305369
1	2.731594	-0.620902	-0.217735
1	1.948188	0.908916	-0.890950
1	0.680265	-1.201367	0.940347
1	-0.366201	1.441585	-0.264136
1	-0.800456	0.834387	1.323943
6	-1.723991	-0.251407	-0.294463
1	-1.924013	-1.166983	0.268089
1	-1.521678	-0.536999	-1.328880
1	-2.634962	0.351779	-0.281302

1-Butene (*AC*), core-ionized state, C1*:

6	1.829302	-0.012583	-0.272014
6	0.701324	-0.266585	0.339123
6	-0.508763	0.558554	0.259513
1	2.646704	-0.634006	-0.187134
1	1.950746	0.823526	-0.862541
1	0.667394	-1.174523	0.939109
1	-0.344712	1.457917	-0.335348
1	-0.736527	0.865376	1.290476
6	-1.711131	-0.272237	-0.269290
1	-1.906521	-1.143216	0.357310
1	-1.545607	-0.601801	-1.294579
1	-2.595864	0.363835	-0.251292

1-Butene (*AC*), core-ionized state, C2*:

6	1.822985	-0.022802	-0.276088
6	0.718735	-0.244445	0.354523
6	-0.534370	0.557404	0.253806
1	2.676074	-0.679095	-0.136046
1	1.905709	0.823622	-0.950971
1	0.671018	-1.060305	0.986007
1	-0.328104	1.408994	-0.394033
1	-0.743243	0.938190	1.256268
6	-1.701156	-0.286809	-0.263622
1	-1.920510	-1.126491	0.398337

1	-1.507161	-0.667482	-1.266830
1	-2.590948	0.342485	-0.304445

1-Butene (*AC*), core-ionized state, C3*:

6	1.820734	0.092704	-0.274787
6	0.722581	-0.382601	0.285788
6	-0.522536	0.429627	0.394688
1	2.701271	-0.533853	-0.338849
1	1.900170	1.093801	-0.684486
1	0.619140	-1.376539	0.699084
1	-0.340612	1.381156	0.030949
1	-0.768386	0.549349	1.394777
6	-1.713638	-0.170159	-0.337146
1	-1.911492	-1.157327	0.074227
1	-1.464485	-0.249180	-1.392149
1	-2.578453	0.475169	-0.194809

1-Butene (*AC*), core-ionized state, C4*:

6	1.814195	0.026829	-0.312153
6	0.721371	-0.302638	0.370941
6	-0.530392	0.521526	0.347594
1	2.716407	-0.569212	-0.243438
1	1.861639	0.905886	-0.946543
1	0.722319	-1.173036	1.021909
1	-0.407086	1.442022	-0.220902
1	-0.883546	0.772581	1.348642
6	-1.691700	-0.253586	-0.323662
1	-1.878150	-1.141122	0.176736
1	-1.446153	-0.491240	-1.301576
1	-2.566278	0.301336	-0.331150

Trans-2-pentene (*AC*), ground state:

```
c
c   1 cc2
h   1 hc3       2 hcc3
h   2 hc4       1 hcc4       3 dih4
c   1 cc5       2 ccc5       4 dih5
c   2 cc6       1 ccc6       5 dih6
h   5 hc7       1 hcc7       3 dih7
h   5 hc8       1 hcc8       3 dih8
h   5 hc9       1 hcc9       3 dih9
h   6 hc10      2 hcc10      4 dih10
h   6 hc11      2 hcc11      4 dih11
c   6 cc12      2 ccc12      1 dih12
h  12 hc13      6 hcc13      11 dih13
h  12 hc14      6 hcc14      10 dih14
h  12 hc15      6 hcc15      2 dih15
```

cc2	1.333
hc3	1.0873
hcc3	119.3174
hc4	1.0897
hcc4	118.0822
dih4	180.0
cc5	1.5017
ccc5	124.8399
dih5	0.0
cc6	1.5063
ccc6	127.1327
dih6	180.0
hc7	1.0947
hcc7	111.2541
dih7	59.3338
hc8	1.0947
hcc8	111.2541
dih8	-59.3338
hc9	1.092
hcc9	111.6011
dih9	180.0
hc10	1.0969
hcc10	108.3095
dih10	-56.5617
hc11	1.0969
hcc11	108.3095
dih11	56.5617
cc12	1.5295
ccc12	116.0959
dih12	0.0
hc13	1.0925
hcc13	111.5277
dih13	183.1498
hc14	1.0925
hcc14	111.5277
dih14	176.8502
hc15	1.0925
hcc15	110.5116
dih15	180.0

Trans-2-pentene (*AC*), core-ionized state, C1*:

c			
c	1 cc2		
h	1 hc3	2 hcc3	
h	2 hc4	1 hcc4	3 dih4
c	1 cc5	2 ccc5	4 dih5
c	2 cc6	1 ccc6	5 dih6
h	5 hc7	1 hcc7	3 dih7

```
h   5 hc8       1 hcc8       3 dih8
h   5 hc9       1 hcc9       3 dih9
h   6 hc10      2 hcc10      4 dih10
h   6 hc11      2 hcc11      4 dih11
c   6 cc12      2 ccc12      1 dih12
h  12 hc13      6 hcc13      11 dih13
h  12 hc14      6 hcc14      10 dih14
h  12 hc15      6 hcc15      2 dih15

      cc2       1.3279
      hc3       1.0796
      hcc3      125.8768
      hc4       1.0896
      hcc4      119.2854
      dih4      180.0
      cc5       1.4994
      ccc5      121.0437
      dih5      0.0
      cc6       1.4962
      ccc6      125.1703
      dih6      180.0
      hc7       1.0384
      hcc7      111.723
      dih7      60.1943
      hc8       1.0384
      hcc8      111.723
      dih8      -60.1943
      hc9       1.0364
      hcc9      110.8944
      dih9      180.0
      hc10      1.0967
      hcc10     106.9754
      dih10     -55.7406
      hc11      1.0967
      hcc11     106.9754
      dih11     55.7406
      cc12      1.5278
      ccc12     116.5907
      dih12     0.0
      hc13      1.0923
      hcc13     111.8691
      dih13     183.4686
      hc14      1.0923
      hcc14     111.8691
      dih14     176.5314
      hc15      1.0905
      hcc15     109.7511
      dih15     180.0
```

Trans-2-pentene (*AC*), core-ionized state, C2*:

```
c
c   1 cc2
h   1 hc3       2 hcc3
h   2 hc4       1 hcc4       3 dih4
c   1 cc5       2 ccc5       4 dih5
c   2 cc6       1 ccc6       5 dih6
h   5 hc7       1 hcc7       3 dih7
h   5 hc8       1 hcc8       3 dih8
h   5 hc9       1 hcc9       3 dih9
h   6 hc10      2 hcc10      4 dih10
h   6 hc11      2 hcc11      4 dih11
c   6 cc12      2 ccc12      1 dih12
h  12 hc13      6 hcc13      11 dih13
h  12 hc14      6 hcc14      10 dih14
h  12 hc15      6 hcc15      2 dih15

      cc2       1.3029
      hc3       1.0312
      hcc3      117.568
      hc4       1.0886
      hcc4      116.7767
      dih4      180.0
      cc5       1.4789
      ccc5      126.3055
      dih5      0.0
      cc6       1.4743
      ccc6      125.1085
      dih6      180.0
      hc7       1.0901
      hcc7      109.4988
      dih7      59.7456
      hc8       1.0901
      hcc8      109.4988
      dih8      -59.7456
      hc9       1.088
      hcc9      109.8111
      dih9      180.0
      hc10      1.1004
      hcc10     105.6529
      dih10     -54.359
      hc11      1.1004
      hcc11     105.6529
      dih11     54.359
      cc12      1.5261
      ccc12     117.3792
      dih12     0.0
      hc13      1.0926
      hcc13     111.979
      dih13     183.9587
```

hc14 1.0926
hcc14 111.979
dih14 176.0413
hc15 1.0899
hcc15 109.451
dih15 180.0

Trans-2-pentene (*AC*), core-ionized state, C3*:

```
c
c   1 cc2
h   1 hc3       2 hcc3
h   2 hc4       1 hcc4       3 dih4
c   1 cc5       2 ccc5       4 dih5
c   2 cc6       1 ccc6       5 dih6
h   5 hc7       1 hcc7       3 dih7
h   5 hc8       1 hcc8       3 dih8
h   5 hc9       1 hcc9       3 dih9
h   6 hc10      2 hcc10      4 dih10
h   6 hc11      2 hcc11      4 dih11
c   6 cc12      2 ccc12      1 dih12
h  12 hc13      6 hcc13      11 dih13
h  12 hc14      6 hcc14      10 dih14
h  12 hc15      6 hcc15      2 dih15

      cc2       1.3013
      hc3       1.0866
      hcc3      116.8721
      hc4       1.0308
      hcc4      117.7861
      dih4      180.0
      cc5       1.4721
      ccc5      124.7256
      dih5      0.0
      cc6       1.4939
      ccc6      127.4502
      dih6      180.0
      hc7       1.0965
      hcc7      108.762
      dih7      57.1139
      hc8       1.0965
      hcc8      108.762
      dih8      -57.1139
      hc9       1.0889
      hcc9      113.8365
      dih9      180.0
      hc10      1.0926
      hcc10     106.4227
      dih10     -56.8896
      hc11      1.0926
```

hcc11 106.4227
dih11 56.8896
cc12 1.5201
ccc12 114.5324
dih12 0.0
hc13 1.0921
hcc13 112.3774
dih13 182.5119
hc14 1.0921
hcc14 112.3774
dih14 177.4881
hc15 1.0904
hcc15 108.0625
dih15 180.0

Trans-2-pentene (*AC*), core-ionized state, C4*:

c
c 1 cc2
h 1 hc3 2 hcc3
h 2 hc4 1 hcc4 3 dih4
c 1 cc5 2 ccc5 4 dih5
c 2 cc6 1 ccc6 5 dih6
h 5 hc7 1 hcc7 3 dih7
h 5 hc8 1 hcc8 3 dih8
h 5 hc9 1 hcc9 3 dih9
h 6 hc10 2 hcc10 4 dih10
h 6 hc11 2 hcc11 4 dih11
c 6 cc12 2 ccc12 1 dih12
h 12 hc13 6 hcc13 11 dih13
h 12 hc14 6 hcc14 10 dih14
h 12 hc15 6 hcc15 2 dih15

cc2 1.3265
hc3 1.0856
hcc3 120.4061
hc4 1.082
hcc4 123.9969
dih4 180.0
cc5 1.4932
ccc5 123.4176
dih5 0.0
cc6 1.4992
ccc6 123.9717
dih6 180.0
hc7 1.0935
hcc7 109.9788
dih7 58.5606
hc8 1.0935
hcc8 109.9788

dih8 -58.5606
hc9 1.0896
hcc9 112.5586
dih9 180.0
hc10 1.0363
hcc10 108.1973
dih10 -56.9565
hc11 1.0363
hcc11 108.1973
dih11 56.9565
cc12 1.5119
ccc12 117.6846
dih12 0.0
hc13 1.0869
hcc13 109.0622
dih13 183.368
hc14 1.0869
hcc14 109.0622
dih14 176.632
hc15 1.0882
hcc15 108.444
dih15 180.0

Trans-2-pentene (*AC*), core-ionized state, C5*:

c
c 1 cc2
h 1 hc3 2 hcc3
h 2 hc4 1 hcc4 3 dih4
c 1 cc5 2 ccc5 4 dih5
c 2 cc6 1 ccc6 5 dih6
h 5 hc7 1 hcc7 3 dih7
h 5 hc8 1 hcc8 3 dih8
h 5 hc9 1 hcc9 3 dih9
h 6 hc10 2 hcc10 4 dih10
h 6 hc11 2 hcc11 4 dih11
c 6 cc12 2 ccc12 1 dih12
h 12 hc13 6 hcc13 11 dih13
h 12 hc14 6 hcc14 10 dih14
h 12 hc15 6 hcc15 2 dih15

cc2 1.3327
hc3 1.0912
hcc3 120.7879
hc4 1.086
hcc4 119.7364
dih4 180.0
cc5 1.4965
ccc5 124.788
dih5 0.0

cc6	1.5005
ccc6	127.7374
dih6	180.0
hc7	1.0936
hcc7	110.6035
dih7	58.9823
hc8	1.0936
hcc8	110.6035
dih8	-58.9823
hc9	1.09
hcc9	111.891
dih9	180.0
hc10	1.092
hcc10	111.6896
dih10	-60.1796
hc11	1.092
hcc11	111.6896
dih11	60.1796
cc12	1.5279
ccc12	112.7085
dih12	0.0
hc13	1.0367
hcc13	110.4708
dih13	182.2428
hc14	1.0367
hcc14	110.4708
dih14	177.7572
hc15	1.0354
hcc15	111.3969
dih15	180.0

Trans-3-hexene (+*AC*+*AC*), ground state:

C
H,1,B1
C,1,B2,2,A1
H,3,B3,1,A2,2,D1,0
C,3,B4,1,A3,2,D2,0
H,5,B5,3,A4,1,D3,0
H,5,B6,3,A5,1,D4,0
C,1,B7,3,A6,5,D5,0
H,8,B8,1,A7,3,D6,0
H,8,B9,1,A8,3,D7,0
C,5,B10,3,A9,1,D8,0
H,11,B11,5,A10,3,D9,0
H,11,B12,5,A11,3,D10,0
H,11,B13,5,A12,3,D11,0
C,8,B14,1,A13,3,D12,0
H,15,B15,8,A14,1,D13,0
H,15,B16,8,A15,1,D14,0

H,15,B17,8,A16,1,D15,0

Variables:

B1	1.0904
B2	1.333
B3	1.0904
B4	1.5033
B5	1.094
B6	1.0962
B7	1.5033
B8	1.094
B9	1.0962
B10	1.5374
B11	1.0932
B12	1.0929
B13	1.0922
B14	1.5374
B15	1.0932
B16	1.0929
B17	1.0922
A1	118.6544
A2	118.6241
A3	125.4822
A4	109.5656
A5	109.2919
A6	125.4693
A7	109.5663
A8	109.2922
A9	112.77
A10	111.1943
A11	111.1296
A12	110.9951
A13	112.7718
A14	111.196
A15	111.1274
A16	110.9958
D1	179.3347
D2	0.0938
D3	-3.7253
D4	-119.978
D5	-179.1446
D6	-3.7226
D7	-119.9751
D8	118.9463
D9	58.1503
D10	178.1072
D11	-61.5808
D12	118.9488
D13	58.1512
D14	178.1069
D15	-61.5823

Trans-3-hexene (+*AC*+*AC*), core-ionized state, C1*:

6	0.577541	-0.470078	0.337703
1	0.551544	-0.467397	1.427935
6	-0.578034	-0.469047	-0.333735
1	-0.579167	-0.500194	-1.421047
6	-1.909589	-0.510488	0.343884
1	-1.821680	-0.639675	1.421735
1	-2.562523	-1.290797	-0.049681
6	1.939967	-0.488949	-0.278601
1	1.859908	-0.519809	-1.367965
1	2.435511	-1.416971	0.027791
6	-2.688257	0.819846	0.132621
1	-2.821664	1.002814	-0.877523
1	-3.619540	0.796405	0.584461
1	-2.148665	1.610577	0.526645
6	2.802486	0.705308	0.165909
1	2.916274	0.734491	1.252022
1	3.800409	0.630664	-0.268526
1	2.367913	1.653498	-0.156086

Trans-3-hexene (+*AC*+*AC*), core-ionized state, C2*:

6	-0.578695	-0.471128	-0.339412
1	-0.553300	-0.467098	-1.429237
6	0.560846	-0.472961	0.342499
1	0.637558	-0.470343	1.421420
6	1.886437	-0.475579	-0.340653
1	1.735089	-0.531733	-1.362418
1	2.406778	-1.334075	-0.083885
6	-1.936922	-0.457172	0.287309
1	-1.850120	-0.498505	1.375419
1	-2.458350	-1.368693	-0.024243
6	2.749154	0.733680	-0.025943
1	2.915001	0.770255	1.048251
1	3.699905	0.640846	-0.548048
1	2.220831	1.626618	-0.349683
6	-2.762169	0.768183	-0.144114
1	-2.887554	0.805774	-1.228463
1	-3.756183	0.720870	0.302315
1	-2.292958	1.699046	0.178301

Trans-3-hexene (+*AC*+*AC*), core-ionized state, C3*:

6	-0.559513	-0.469936	-0.333219
1	-0.529931	-0.464555	-1.363703
6	0.571020	-0.471457	0.313831
1	0.509785	-0.467325	1.401155
6	1.908899	-0.462896	-0.306366

1	1.841842	-0.495311	-1.395356
1	2.410332	-1.381801	0.026161
6	-1.921254	-0.459464	0.270991
1	-1.800843	-0.534289	1.351918
1	-2.431241	-1.363451	-0.068233
6	2.742537	0.750246	0.175649
1	2.850530	0.758384	1.261334
1	3.738909	0.683131	-0.261043
1	2.294805	1.692434	-0.140271
6	-2.709003	0.790534	-0.121407
1	-2.845708	0.860478	-1.202271
1	-3.699176	0.740922	0.333178
1	-2.219331	1.699676	0.229948

1,5-hexadiene (*skew*), ground state:

6	2.596499	-0.672627	0.185149
6	1.392584	-0.402738	-0.315224
6	0.712610	0.934864	-0.246228
6	-0.663165	0.893807	0.463286
6	-1.710297	0.133157	-0.299887
6	-2.363714	-0.938792	0.142905
1	0.836784	-1.196739	-0.808705
1	3.036983	-1.660074	0.105077
1	3.188146	0.083992	0.691337
1	1.361080	1.649262	0.268634
1	0.566424	1.320625	-1.262921
1	-0.548400	0.470356	1.464805
1	-1.003851	1.928120	0.591513
1	-1.936475	0.510974	-1.296216
1	-2.172858	-1.356285	1.126453
1	-3.114939	-1.436251	-0.459978

1,5-hexadiene (*skew*), core-ionized state, C1*:

6	2.560475	-0.692326	0.136957
6	1.339595	-0.400833	-0.233774
6	0.745236	0.936841	-0.214594
6	-0.674362	0.924547	0.452091
6	-1.683075	0.130095	-0.328198
6	-2.316911	-0.945176	0.135126
1	0.714776	-1.226716	-0.571230
1	2.920358	-1.656977	0.108112
1	3.216105	0.029849	0.469437
1	1.409600	1.671641	0.243494
1	0.606162	1.219386	-1.270012
1	-0.597386	0.564153	1.480028
1	-0.976136	1.974427	0.505612
1	-1.914592	0.497965	-1.325603
1	-2.143120	-1.332213	1.134606

1	-3.061523	-1.460402	-0.460092

1,5-hexadiene (*skew*), core-ionized state, C2*:

6	2.467914	-0.741286	0.111065
6	1.272880	-0.378245	-0.210125
6	0.714573	0.999167	-0.199280
6	-0.694234	0.995374	0.429838
6	-1.644017	0.109979	-0.331881
6	-2.154207	-1.027309	0.140530
1	0.579043	-1.097301	-0.492289
1	2.749726	-1.788796	0.073674
1	3.201502	-0.003131	0.420802
1	1.405901	1.650100	0.335729
1	0.663108	1.331491	-1.239997
1	-0.630502	0.690912	1.477119
1	-1.041845	2.032274	0.416236
1	-1.918887	0.443728	-1.330280
1	-1.943064	-1.381627	1.145156
1	-2.842440	-1.623730	-0.447040

1,5-hexadiene (*skew*), core-ionized state, C3*:

6	2.573706	-0.631618	0.180909
6	1.367220	-0.429048	-0.320132
6	0.704246	0.898842	-0.255480
6	-0.665076	0.893958	0.473748
6	-1.708673	0.152391	-0.304640
6	-2.311655	-0.943369	0.148007
1	0.762134	-1.182824	-0.803235
1	3.020664	-1.615462	0.116999
1	3.160079	0.142651	0.663642
1	1.329879	1.572771	0.217123
1	0.555751	1.261855	-1.214801
1	-0.486227	0.451980	1.452601
1	-0.930854	1.945622	0.602146
1	-2.010211	0.589335	-1.253751
1	-2.058829	-1.390596	1.103670
1	-3.100997	-1.422271	-0.418868

1,5-hexadiene (*skew*), core-ionized state, C4*:

6	2.513702	-0.682019	0.214367
6	1.370094	-0.376310	-0.393250
6	0.712312	0.961384	-0.246268
6	-0.653284	0.855584	0.483140
6	-1.713986	0.155123	-0.285222
6	-2.270490	-0.965085	0.142089
1	0.895418	-1.087865	-1.060944
1	2.989063	-1.643395	0.060224

1	3.030148	0.014092	0.867505
1	1.320582	1.646816	0.344079
1	0.494455	1.428590	-1.208137
1	-0.498816	0.370835	1.383774
1	-0.972120	1.813872	0.713160
1	-1.970944	0.655015	-1.209428
1	-1.996785	-1.450221	1.072376
1	-3.041086	-1.439807	-0.451736

1,5-hexadiene (*skew*), core-ionized state, C5*:

6	2.236333	-0.760789	0.295254
6	1.304525	-0.246027	-0.507352
6	0.635755	1.082836	-0.279551
6	-0.700835	0.971928	0.503613
6	-1.665501	0.083022	-0.186232
6	-1.860648	-1.165575	0.092834
1	1.020009	-0.796029	-1.401335
1	2.702603	-1.715120	0.079691
1	2.589230	-0.239060	1.179443
1	1.271688	1.736262	0.322627
1	0.460889	1.599451	-1.226977
1	-0.524209	0.563612	1.497705
1	-1.169034	1.951675	0.607204
1	-2.159808	0.488347	-0.996160
1	-1.352778	-1.618982	0.937136
1	-2.536364	-1.762530	-0.510720

1,5-hexadiene (*skew*), core-ionized state, C6*:

6	2.436090	-0.685208	0.260979
6	1.353536	-0.341317	-0.433794
6	0.664661	0.984999	-0.303647
6	-0.694454	0.910165	0.513081
6	-1.691631	0.136874	-0.220665
6	-2.112980	-1.056703	0.118819
1	0.949605	-1.040605	-1.163187
1	2.920132	-1.643745	0.114982
1	2.892419	-0.017033	0.984292
1	1.285257	1.691862	0.249653
1	0.464618	1.428848	-1.282344
1	-0.505435	0.500788	1.505443
1	-1.066773	1.936764	0.601470
1	-2.097314	0.550332	-1.142125
1	-1.778800	-1.523587	0.974188
1	-2.795041	-1.576481	-0.451005