Suppementary material and supporting information for

PREDICTIONS OF ^{13}C CHEMICAL SHIFTS IN CARBOCATIONS. THE USE OF SCALED CHEMICAL SHIFTS CALCULATED USING GIAO DFT METHODS.

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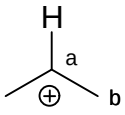
Structures for table S1 and S2



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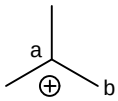

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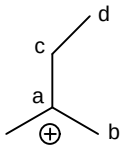
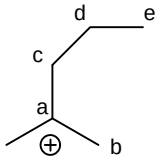


3A/3B



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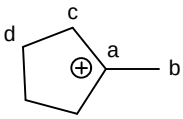

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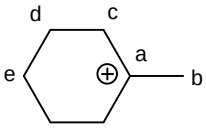

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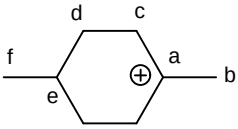
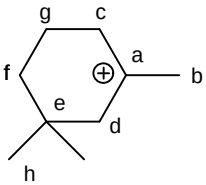


7A/7B



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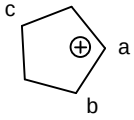

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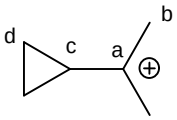

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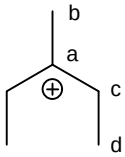

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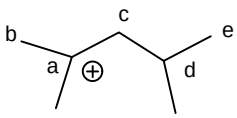
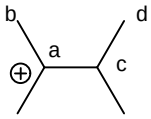


12



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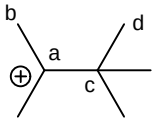

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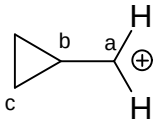

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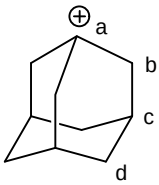

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Table S1. Experimental[a] and Calculated ^{13}C NMR Shifts GIAO-B3LYP/6-311G(d,p)// B3LYP-6/31G(d) and GIAO-B3LYP/6-311G(d,p)// MP2/6-31G(d). Calculations for C-H Hyperconjugative Isomers of Carbocations (Group **A**).

carbocation	carbon atom	d_{calc}/ppm DFT[b]	d_{calc}/ppm MP[c]	d_{exp}/ppm	d_{exp}/d_{calc} DFT	d_{exp}/d_{calc} MP
	a	339.10	333.51	320.6	0.95	0.96
1	b	57.40	58.20	51.5	0.90	0.88
	a	351.73	346.00	335	0.95	0.97
2	b	52.12	51.51	47.5	0.91	0.92
	a	353.59	350.46	335.4	0.95	0.96
3A	b	49.37	51.78	44.6	0.90	0.86
	c	65.87	65.67	57.5	0.87	0.88
	d	12.00	12.26	9.3	0.78	0.76
	a	350.88	347.91	333.4	0.95	0.96
	b	49.28	48.89	45.0	0.91	0.92
4A	c	74.30	73.60	64.4	0.91	0.88
	d	25.20	24.78	20.9	0.83	0.84
	e	13.94	13.84	12.6	0.90	0.91
	a	354.35	350.52	336.9	0.95	0.96
	b	41.54	41.62	36.7	0.88	0.88
5	c	70.15	70.09	63.3	0.90	0.90
	d	31.62	31.75	26.4	0.83	0.83
	a	350.92	346.91	332.7	0.95	0.96
	b	50.76	50.83	44.2	0.87	0.87
6	c	64.69	64.66	58.2	0.90	0.90
	d	32.98	31.64	26.9	0.82	0.85
	e	26.44	26.52	22.2	0.84	0.84
	a	348.97	344.77	328.7	0.94	0.95
	b	49.57	49.64	43.6	0.88	0.88
7	c	63.84	63.68	56.4	0.88	0.89
	d	46.86	44.37	35.8	0.76	0.81
	e	38.85	36.33	29.5	0.76	0.81
	f	28.61	29.11	27.3	0.95	0.94
	a	346.89	343.73	329.0	0.95	0.96
	b	48.50	49.08	46.2	0.94	0.94
	c	80.40	79.48	69.7	0.87	0.88
8	d	65.55	65.13	58.6	0.89	0.90
	e	31.86	34.52	26.1	0.82	0.76
	f	42.98	44.13	35.0	0.81	0.79
	g	74.88	75.86	43.5	0.58	0.57
	h	35.62	35.62	29.1	0.82	0.82
	a	336.15	330.20	320.0	0.95	0.97
9	b	76.46	76.69	71.0	0.92	0.92
	c	31.39	31.43	28.0	0.89	0.89
	a	294.19	290.17	279.3	0.95	0.96
	b	37.73	37.39	34.1	0.90	0.91
10	c	61.87	61.44	57.3	0.94	0.93
	d	60.51	61.35	54.15	0.89	0.88

[a] Experimental chemical shifts are taken from Ref. 10.a. (**1**, **2**, **3A** and **4A**), Ref. 13 (**5**), Ref. 14 (**6**), ref. 15 (**7**, **8**), Ref. 16 (**9**) and Ref. 17 (**10**).
[b] Calculated ^{13}C NMR shifts from GIAO-B3LYP/6-311G(d,p)// B3LYP-6/31G(d) method.
[c] Calculated ^{13}C NMR shifts from GIAO-B3LYP/6-311G(d,p)// MP2-6/31G(d) method.

Table S2. Experimental[a] and Calculated ^{13}C NMR Shifts from GIAO B3LYP/6-311G(d,p)// B3LYP-6/31G(d) and from GIAO B3LYP/6-311G(d,p)//MP2-6/31G(d) Calculations for C-C Hyperconjugative Isomers of Carbocations (Group **B**).

carbocation	carbon atom	d_{calc}/ppm DFT	d_{calc}/ppm MP	d_{exp}/ppm	d_{exp}/ d_{calc} DFT	d_{exp}/ d_{calc} MP
3B	a	344.90	333.06	335.4	0.97	1.01
	b	48.17	46.98	44.6	0.93	0.95
	c	63.05	62.83	57.5	0.91	0.92
	d	25.99	23.96	9.3	0.36	0.39
4B	a	343.98	319.17	333.4	0.97	1.04
	b	46.92	44.74	45.0	0.95	1.01
	c	73.52	73.53	64.4	0.88	0.88
	d	47.47	44.16	20.9	0.53	0.47
	e	23.73	23.83	12.6	0.44	0.53
11	a	345.51	334.30	336.4	0.97	1.01
	b	45.24	43.80	41.9	0.92	0.96
	c	59.51	58.69	54.5	0.91	0.93
	d	13.79	24.64	8.9	0.65	0.36
12	a	337.8	331.70	332.1	0.98	1.00
	b	48.07	47.55	45.4	0.94	0.95
	c	80.04	79.44	70.1	0.88	0.88
	d	67.54	63.52	31.4	0.47	0.49
	e	29.67	25.20	21.7	0.73	0.86
13	a	343.12	330.69	335	0.97	1.01
	b	45.78	44.37	43	0.94	0.97
	c	66.67	62.65	59	0.89	0.94
	d	27.16	26.56	17	0.63	0.64
14	a	342.00	323.97	330	0.97	1.02
	b	45.17	42.99	41	0.91	0.95
	c	68.45	67.87	56	0.82	0.83
	d	32.41	31.96	n.a.	-	-
15	a	242.69	245.08	235	0.97	0.96
	b	80.35	86.22	n.a.	-	-
	c	84.49	85.09	n.a.	-	-
16	a	310.60	305.89	300	0.97	0.98
	b	72.54	71.50	65.7	0.91	0.92
	c	102.63	100.23	86.8	0.85	0.87
	d	41.89	41.64	34.5	0.82	0.83

[a] Experimental chemical shifts are taken from Ref. 10.a. (**3B**, **4B**, **11** and **12**), Ref. 16 (**13**, **14**), Ref. 18. (**15**) and Ref 19. (**16**).

Optimized structures of carbocations **1** - **16** in Gaussian z-matrix format

Isopropyl cation **1**

E (B3LYP/6-31G(d)) = -118.2117339 Hartree
E (B3LYP/6-31G(d)) + ZPE = -118.1124134 Hartree
NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:
C
C,1,r2
H,2,r3,1,a3
H,2,r4,1,a4,3,d4,0
H,2,r5,1,a5,3,d5,0
H,1,r6,2,a6,3,d6,0
H,1,r7,2,a7,3,d7,0
C,7,r8,1,a8,2,d8,0
H,8,r9,7,a9,1,d9,0
H,8,r10,7,a10,1,d10,0
Variables:
r2=1.44294135
r3=1.10912749
a3=108.10220158
r4=1.10928782
a4=108.0339845
d4=-108.58850267
r5=1.08982167
a5=115.4867559
d5=125.76261484
r6=1.09446821
a6=116.68676347
d6=54.16230466
r7=2.15014703
a7=99.39832871
d7=-125.83298226
r8=1.08982159
a8=37.28514096
d8=-179.8886148
r9=1.10929014
a9=111.53251847
d9=123.83159863
r10=1.10912546
a10=111.57724709
d10=-123.96503301

Isopropyl cation **1**

E (MP2/6-31G(d)) = - 117.7466525 Hartree
E (MP2/6-31G(d)) + ZPE = -117.6559325 Hartree
NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
H,2,R7,1,A7,6,D7,0
H,6,R8,2,A8,1,D8,0
H,6,R9,2,A9,8,D9,0
H,6,R10,2,A10,8,D10,0
Variables:
R2=1.43902238
R3=1.08964777
R4=1.11757304
R5=1.09446505
R6=1.43902218
R7=1.09296681
R8=1.11757402
R9=1.09446824
R10=1.08964839
A3=114.92501639
A4=101.02258304
A5=113.21353219
A6=125.45204578
A7=117.27390587
A8=101.02342289
A9=113.21368966
A10=114.92487802
D4=-115.9448533
D5=133.41475192
D6=12.75375373
D7=-179.99973971
D8=-103.1877104
D9=-110.64095387
D10=115.94486488

t-butyl cation **2**

E (B3LYP/6-31G(d)) = -157.5540581 Hartree
E (B3LYP/6-31G(d)) + ZPE = -157.4375667 Hartree
NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:
C
C,1,r2
C,2,r3,1,a3
C,2,r4,1,a4,3,d4,0
H,3,r5,2,a5,1,d5,0
H,1,r6,2,a6,3,d6,0
H,1,r7,2,a7,3,d7,0
H,1,r8,2,a8,3,d8,0
H,4,r9,2,a9,1,d9,0
H,4,r10,2,a10,1,d10,0
H,4,r11,2,a11,1,d11,0
H,3,r12,2,a12,1,d12,0
H,3,r13,2,a13,1,d13,0
Variables:
r2=1.4664639
r3=1.46657356
a3=120.66882316
r4=1.46504218
a4=119.66231962
d4=-178.20280596
r5=1.09242378
a5=113.83478448
d5=26.51385465
r6=1.11048398
a6=104.87257676
d6=90.12569437
r7=1.09238138
a7=113.86578622
d7=-26.24748922
r8=1.09495932
a8=112.87233546
d8=-155.77308652
r9=1.09383
a9=113.61094461
d9=23.5828535
r10=1.11119302
a10=104.07860446
d10=-91.36719769
r11=1.09405144
a11=113.5463901
d11=153.86997076
r12=1.11044266
a12=104.89017451
d12=-89.81695885
r13=1.09490937
a13=112.89291521
d13=156.01651576

t-butyl cation **2**

E (MP2/6-31G(d)) = -156.9407116 Hartree
E (MP2/6-31G(d)) + ZPE = -156.8296776 Hartree
NImag = 0

Final MP2/6-31G(d) structure in terms of inital Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
H,6,R8,2,A8,1,D8,0
H,7,R9,2,A9,1,D9,0
H,7,R10,2,A10,9,D10,0
H,7,R11,2,A11,9,D11,0
H,6,R12,2,A12,8,D12,0
H,6,R13,2,A13,8,D13,0
Variables:
R2=1.46155664
R3=1.10849922
R4=1.09027439
R5=1.09281934
R6=1.46160928
R7=1.45991271
R8=1.09033582
R9=1.09180092
R10=1.10931672
R11=1.09193385
R12=1.1084909
R13=1.09274307
A3=104.060751
A4=113.65184889
A5=112.66645538
A6=120.71614414
A7=119.62418249
A8=113.61798612
A9=113.4292664
A10=103.22079952
A11=113.37838597
A12=104.06421966
A13=112.69962709
D4=-116.40646071
D5=114.25977879
D6=89.83911592
D7=-177.49719126
D8=26.91914275
D9=23.44500149
D10=-114.97981329
D11=130.16168877
D12=-116.33253247
D13=129.33475441

2-methyl-2-butyl cation **3A**

E (B3LYP/6-31G(d)) = -196.9715415 Hartree
E (B3LYP/6-31G(d)) + ZPE = -196.8356466 Hartree
NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:
H
C,1,r2
H,2,r3,1,a3
C,2,r4,1,a4,3,d4,0
H,2,r5,1,a5,3,d5,0
C,4,r6,2,a6,1,d6,0
H,6,r7,4,a7,2,d7,0
C,4,r8,2,a8,1,d8,0
H,8,r9,4,a9,2,d9,0
H,8,r10,4,a10,2,d10,0
H,8,r11,4,a11,2,d11,0
H,6,r12,4,a12,2,d12,0
H,6,r13,4,a13,2,d13,0
C,7,r14,6,a14,4,d14,0
H,14,r15,7,a15,6,d15,0
H,14,r16,7,a16,6,d16,0
Variables:
r2=1.09106683
r3=1.10227409
a3=110.45177888
r4=1.46956804
a4=114.41916733
d4=-123.54943619
r5=1.10348095
a5=110.04053266
d5=114.0980686
r6=1.46928189
a6=119.40804202
d6=-1.11641996
r7=2.18596854
a7=104.31096823
d7=156.65195973
r8=1.46544107
a8=119.45616147
d8=178.8335037
r9=1.10325843
a9=108.82097882
d9=-124.01028828
r10=1.10308464
a10=108.86788164
d10=124.10123504
r11=1.09039979
a11=114.39723457
d11=-0.03170164
r12=1.10946479
a12=104.68592939
d12=54.86798815
r13=1.10794178
a13=105.4996914
d13=-50.92097839
r14=1.09460847
a14=40.34202653
d14=128.64806001
r15=1.09260556
a15=107.47762061
d15=119.95027319
r16=1.09472135
a16=108.59747517
d16=-124.04979584

2-methyl-2-butyl cation **3A**

E (MP2/6-31G(d)) = - 196.1098651 Hartree

E (MP2/6-31G(d)) + ZPE = -195.9606691 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of inital Z-matrix:

H
C,1,R2
H,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,4,R7,2,A7,6,D7,0
H,7,R8,4,A8,2,D8,0
H,7,R9,4,A9,8,D9,0
H,7,R10,4,A10,8,D10,0
H,6,R11,4,A11,2,D11,0
C,6,R12,4,A12,11,D12,0
H,6,R13,4,A13,11,D13,0
H,12,R14,6,A14,4,D14,0
H,12,R15,6,A15,14,D15,0
H,12,R16,6,A16,14,D16,0
Variables:
R2=1.10616408
R3=1.09003462
R4=1.4632242
R5=1.09562808
R6=1.46184374
R7=1.46191304
R8=1.10364367
R9=1.09776873
R10=1.08911555
R11=1.10112624
R12=1.52193223
R13=1.11305112
R14=1.09111716
R15=1.09262188
R16=1.09178304
A3=108.71992707
A4=105.01206309
A5=105.05518642
A6=119.38340222
A7=119.55399195
A8=107.1786151
A9=109.95904604
A10=113.80560142
A11=108.0691348
A12=119.29896235
A13=101.41738614
A14=109.07306553
A15=111.28173024
A16=112.11192808
D4=-122.4419762
D5=120.03261345
D6=108.45801184
D7=179.0767932
D8=-117.10226835
D9=-112.86929295
D10=121.3218087
D11=-37.60963284
D12=-130.92200592
D13=106.6763967
D14=-177.5752103
D15=-118.58342926
D16=119.09579916

2-methyl-2-butyl cation **3B**

E (B3LYP/6-31G(d)) = -196.8716621 Hartree

E (B3LYP/6-31G(d)) + ZPE = -196.7256411 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,r2
H,2,r3,1,a3
C,2,r4,1,a4,3,d4,0
H,2,r5,1,a5,3,d5,0
C,4,r6,2,a6,1,d6,0
H,6,r7,4,a7,2,d7,0
C,4,r8,2,a8,1,d8,0
H,8,r9,4,a9,2,d9,0
H,8,r10,4,a10,2,d10,0
H,8,r11,4,a11,2,d11,0
H,6,r12,4,a12,2,d12,0
H,6,r13,4,a13,2,d13,0
C,7,r14,6,a14,4,d14,0
H,14,r15,7,a15,6,d15,0
H,14,r16,7,a16,6,d16,0
Variables:
r2=1.09102762
r3=1.10670766
a3=108.45706223
r4=1.46970483
a4=114.05142735
d4=-118.48148687
r5=1.09815878
a5=111.45222359
d5=114.35227168
r6=1.45948686
a6=120.42456331
d6=5.39335749
r7=2.23327161
a7=91.51115421
d7=-107.910863
r8=1.47056496
a8=119.73356092
d8=-174.34624751
r9=1.10812124
a9=105.38037044
d9=-98.6808081
r10=1.09620786
a10=112.10765983
d10=147.88543757
r11=1.09176479
a11=114.29448507
d11=19.44323555
r12=1.09335536
a12=112.43195326
d12=157.66524802
r13=1.09462461
a13=111.67809404
d13=32.16190355
r14=1.09216292
a14=41.33238374
d14=122.13178879
r15=1.09301476
a15=108.83457068
d15=116.47586005
r16=1.09197702
a16=109.7769619
d16=-124.42248799

2-methyl-2-butyl cation **3B**

E (MP2/6-31G(d)) = -196.111144 Hartree

E (MP2/6-31G(d)) + ZPE = -195.9610270 Hartree
NImag = 0
Final MP2/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,4,R7,2,A7,6,D7,0
H,7,R8,4,A8,2,D8,0
H,7,R9,4,A9,8,D9,0
H,7,R10,4,A10,8,D10,0
H,6,R11,4,A11,2,D11,0
H,6,R12,4,A12,11,D12,0
C,6,R13,4,A13,11,D13,0
H,13,R14,6,A14,4,D14,0
H,13,R15,6,A15,14,D15,0
H,13,R16,6,A16,14,D16,0
Variables:
R2=1.08942581
R3=1.10421373
R4=1.46648643
R5=1.09586188
R6=1.44716721
R7=1.46628291
R8=1.10673074
R9=1.09266046
R10=1.09073766
R11=1.09165209
R12=1.09214371
R13=1.58312177
R14=1.0908042
R15=1.09167808
R16=1.09044616
A3=108.79511828
A4=113.6947164
A5=111.54289833
A6=120.49987174
A7=119.60668905
A8=104.16161209
A9=112.54215376
A10=113.8140985
A11=113.14135434
A12=112.77159524
A13=101.70534517
A14=111.84390447
A15=105.49266778
A16=111.697695
D4=-117.86701278
D5=115.4749353
D6=4.50710885
D7=-179.59166282
D8=-92.04586074
D9=-114.32425447
D10=116.85572041
D11=157.89775628
D12=-127.95246134
D13=116.46419624
D14=-60.37712819
D15=-118.04298712
D16=123.80786715

2-methyl-2-pentyl cation **4A**

E (B3LYP/6-31G(d)) = -236.1867547 Hartree

E (B3LYP/6-31G(d)) + ZPE = -236.0121927 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
H,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,5,R6,2,A6,1,D6,0
C,5,R7,2,A7,6,D7,0
C,6,R8,5,A8,2,D8,0
H,7,R9,5,A9,2,D9,0
H,7,R10,5,A10,9,D10,0
H,6,R11,5,A11,8,D11,0
H,6,R12,5,A12,8,D12,0
H,7,R13,5,A13,9,D13,0
C,8,R14,6,A14,5,D14,0
H,8,R15,6,A15,14,D15,0
H,8,R16,6,A16,14,D16,0
H,14,R17,8,A17,6,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
Variables:
R2=1.10197686
R3=1.10425948
R4=1.09010321
R5=1.46651083
R6=1.46788181
R7=1.46967207
R8=1.53341743
R9=1.10674071
R10=1.09172661
R11=1.1151946
R12=1.10399094
R13=1.09917515
R14=1.53305316
R15=1.09773084
R16=1.09691431
R17=1.09303431
R18=1.0954935
R19=1.09549669
A3=103.50327894
A4=110.819399
A5=109.30505566
A6=121.18178646
A7=119.35704749
A8=120.36792457
A9=106.37821403
A10=114.29488282
A11=102.16246795
A12=108.06719833
A13=110.95512895
A14=111.50196709
A15=109.08072207
A16=109.90479037
A17=110.17358127
A18=111.4316537
A19=111.4555591

D4=117.728941
D5=-115.52226429
D6=54.35162628
D7=179.66865892
D8=-11.43494437
D9=68.42648095
D10=120.01971147
D11=122.79631037
D12=-131.07250916
D13=-112.82862966
D14=178.42912695
D15=121.34575118
D16=-121.7892254
D17=178.95082237
D18=-119.53834314
D19=119.54374629

2-methyl-2-pentyl cation **4A**

E (MP2/6-31G(d)) = - 235.2771648 Hartree

E (MP2/6-31G(d)) + ZPE = -235.0986888 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
H,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,5,R6,2,A6,1,D6,0
C,5,R7,2,A7,6,D7,0
C,6,R8,5,A8,2,D8,0
H,7,R9,5,A9,2,D9,0
H,7,R10,5,A10,9,D10,0
H,6,R11,5,A11,8,D11,0
H,6,R12,5,A12,8,D12,0
H,7,R13,5,A13,9,D13,0
C,8,R14,6,A14,5,D14,0
H,8,R15,6,A15,14,D15,0
H,8,R16,6,A16,14,D16,0
H,14,R17,8,A17,6,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
Variables:
R2=1.10154781
R3=1.1037945
R4=1.09047307
R5=1.46725978
R6=1.46739053
R7=1.46932967
R8=1.53306689
R9=1.10686651
R10=1.09145674
R11=1.11505775
R12=1.10406127
R13=1.09871448
R14=1.53317586
R15=1.09774807
R16=1.09655231
R17=1.09315363
R18=1.09562073
R19=1.09563622
A3=103.52815574
A4=110.86603635
A5=109.31439066
A6=121.15707811
A7=119.33640046
A8=120.38715738
A9=106.39930367
A10=114.30918159
A11=102.20742527
A12=108.01692424
A13=110.98801695
A14=111.49271856
A15=109.07785403
A16=109.93343674
A17=110.17498224
A18=111.45046749
A19=111.47172385
D4=117.73958344
D5=-115.52034802
D6=54.37622482
D7=179.62212404
D8=-11.45633695
D9=68.46621703
D10=119.9733647

D11=122.83636409
D12=-131.06984516
D13=-112.8412514
D14=178.45744563
D15=121.2864211
D16=-121.82542576
D17=178.93467613
D18=-119.49073149
D19=119.55918296

2-methyl-2-pentyl cation **4B**

E (B3LYP/6-31G(d)) = -236.1890571 Hartree

E (B3LYP/6-31G(d)) + ZPE = -236.0132941 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
H,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,5,R6,2,A6,1,D6,0
C,5,R7,2,A7,6,D7,0
C,6,R8,5,A8,2,D8,0
H,7,R9,5,A9,2,D9,0
H,7,R10,5,A10,9,D10,0
H,6,R11,5,A11,8,D11,0
H,6,R12,5,A12,8,D12,0
H,7,R13,5,A13,9,D13,0
C,8,R14,6,A14,5,D14,0
H,8,R15,6,A15,14,D15,0
H,8,R16,6,A16,14,D16,0
H,14,R17,8,A17,6,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
Variables:
R2=1.09513936
R3=1.092547
R4=1.10789484
R5=1.47247055
R6=1.45163446
R7=1.47218949
R8=1.60628617
R9=1.10245052
R10=1.09053827
R11=1.0938974
R12=1.09338377
R13=1.10190238
R14=1.53163861
R15=1.09442368
R16=1.09404831
R17=1.09532895
R18=1.09403361
R19=1.09405635
A3=111.74143511
A4=105.3195321
A5=112.47292876
A6=119.97921173
A7=119.15828865
A8=105.32149466
A9=108.6703383
A10=114.13266627
A11=112.3775204
A12=112.77068365
A13=109.33969267
A14=109.06505124
A15=109.15482232
A16=108.99139518
A17=108.48024782
A18=111.6921732
A19=111.61395049
D4=116.1346844
D5=-129.75972166
D6=-28.65403043
D7=178.28371855
D8=94.85752609

D9=53.54931902
D10=123.00649253
D11=116.04927004
D12=-117.10061428
D13=-112.93304485
D14=-178.43515845
D15=121.04247892
D16=-121.10292969
D17=-179.85447633
D18=-118.98891465
D19=119.02417326

2-methyl-2-butyl cation **4B**

E (MP2/6-31G(d)) = -235.2806244 Hartree

E (MP2/6-31G(d)) + ZPE = -235.1008714 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
H,2,R4,1,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,5,R6,2,A6,1,D6,0
C,5,R7,2,A7,6,D7,0
C,6,R8,5,A8,2,D8,0
H,7,R9,5,A9,2,D9,0
H,7,R10,5,A10,9,D10,0
H,6,R11,5,A11,8,D11,0
H,6,R12,5,A12,8,D12,0
H,7,R13,5,A13,9,D13,0
C,8,R14,6,A14,5,D14,0
H,8,R15,6,A15,14,D15,0
H,8,R16,6,A16,14,D16,0
H,14,R17,8,A17,6,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
Variables:
R2=1.09204578
R3=1.09147887
R4=1.10605535
R5=1.46868665
R6=1.43778733
R7=1.46951282
R8=1.6012708
R9=1.10048116
R10=1.08915642
R11=1.09176758
R12=1.09161233
R13=1.09885714
R14=1.52894701
R15=1.09388002
R16=1.09275617
R17=1.09307241
R18=1.09180603
R19=1.09188121
A3=111.91118226
A4=106.39630818
A5=112.73557822
A6=120.11871226
A7=119.01953895
A8=100.48355297
A9=107.9668236
A10=113.66020539
A11=113.83027254
A12=113.8443699
A13=109.41760166
A14=108.06489725
A15=110.25237448
A16=109.09314265
A17=108.64937756
A18=111.35201558
A19=111.21219283
D4=116.87325626
D5=-129.46704691
D6=-23.35374223
D7=177.98892511
D8=94.46198399

D9=54.59305762
D10=122.21154167
D11=114.33289172
D12=-115.37116374
D13=-113.59199987
D14=-174.39085681
D15=120.61725371
D16=-120.50127993
D17=-178.7246577
D18=-119.14161727
D19=119.15045503

methyl_cyclopentyl cation **5**

E (B3LYP/6-31G(d)) = -234.9794440 Hartree

E (B3LYP/6-31G(d)) + ZPE = -234.8248711 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,r2
C,2,r3,1,a3
C,3,r4,2,a4,1,d4,0
C,4,r5,3,a5,2,d5,0
C,2,r6,1,a6,3,d6,0
H,1,r7,2,a7,3,d7,0
H,3,r8,2,a8,1,d8,0
H,3,r9,2,a9,1,d9,0
H,4,r10,3,a10,2,d10,0
H,4,r11,3,a11,2,d11,0
H,5,r12,4,a12,3,d12,0
H,5,r13,4,a13,3,d13,0
H,6,r14,2,a14,1,d14,0
H,6,r15,2,a15,1,d15,0
H,1,r16,2,a16,3,d16,0
H,1,r17,2,a17,3,d17,0
Variables:
r2=1.46424483
r3=1.47021441
a3=125.35325295
r4=1.54616737
a4=106.23147672
d4=-172.40767056
r5=1.54247386
a5=103.09211156
d5=-27.35760672
r6=1.46777586
a6=124.77454186
d6=177.90697661
r7=1.09539014
a7=112.39961724
d7=152.59614296
r8=1.11399525
a8=102.57922761
d8=72.2752284
r9=1.09684395
a9=113.99787027
d9=-39.99666028
r10=1.09565086
a10=109.46786857
d10=90.83548555
r11=1.09131918
a11=112.22121324
d11=-149.63071567
r12=1.09568581
a12=111.09998865
d12=-83.05616393
r13=1.09135334
a13=113.36303394
d13=155.40558748
r14=1.09659596
a14=114.75432396
d14=-31.99344606
r15=1.1155756
a15=101.41598248
d15=80.21812592
r16=1.09268501
a16=113.58136296
d16=24.32382323
r17=1.10789312

a17=105.79518585
d17=-92.96718763

1-methyl-cyclopentyl cation **5**

E (MP2/6-31G(d)) = -234.1085876Hartree

E (MP2/6-31G(d)) + ZPE = -233.9508256 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
C,2,R7,1,A7,3,D7,0
H,2,R8,1,A8,7,D8,0
H,2,R9,1,A9,7,D9,0
H,3,R10,1,A10,6,D10,0
H,3,R11,1,A11,6,D11,0
C,7,R12,2,A12,1,D12,0
H,6,R13,3,A13,1,D13,0
H,6,R14,3,A14,13,D14,0
H,12,R15,7,A15,2,D15,0
H,12,R16,7,A16,15,D16,0
H,12,R17,7,A17,15,D17,0
Variables:
R2=1.53787868
R3=1.53440897
R4=1.09483076
R5=1.09115175
R6=1.5370533
R7=1.4630789
R8=1.11400762
R9=1.09557565
R10=1.09491913
R11=1.09117053
R12=1.46014833
R13=1.11580342
R14=1.09567721
R15=1.09318756
R16=1.09095474
R17=1.10615316
A3=102.64998728
A4=109.66211395
A5=112.28331317
A6=102.44062587
A7=105.80316006
A8=109.40499762
A9=118.99169241
A10=111.00169804
A11=113.46432916
A12=125.37953893
A13=109.01470855
A14=119.49332492
A15=112.20757778
A16=113.30104152
A17=104.94099027
D4=-117.92907442
D5=122.17282248
D6=-36.26090001
D7=29.47436154
D8=-108.81211555
D9=130.29138327
D10=117.00234621
D11=-121.28757643
D12=171.68446695
D13=-76.59765082
D14=-121.1140095
D15=-153.95792215

D16=128.21897754
D17=-114.66966165

1-methyl-cyclohexyl cation **6A**

E (B3LYP/6-31G(d)) = -274.300061 Hartree

E (B3LYP/6-31G(d)) + ZPE = -274.1137065 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,r2
C,2,r3,1,a3
C,3,r4,2,a4,1,d4,0
C,3,r5,2,a5,1,d5,0
C,4,r6,3,a6,2,d6,0
C,3,r7,2,a7,1,d7,0
H,3,r8,2,a8,1,d8,0
H,4,r9,3,a9,2,d9,0
H,5,r10,3,a10,2,d10,0
H,6,r11,4,a11,3,d11,0
H,7,r12,3,a12,2,d12,0
H,2,r13,1,a13,3,d13,0
H,3,r14,2,a14,1,d14,0
H,4,r15,3,a15,2,d15,0
H,5,r16,3,a16,2,d16,0
C,11,r17,6,a17,4,d17,0
H,7,r18,3,a18,2,d18,0
H,17,r19,11,a19,6,d19,0
H,17,r20,11,a20,6,d20,0
Variables:
r2=1.09669877
r3=2.54983561
a3=147.42357319
r4=2.54984165
a4=59.92890859
d4=135.40990551
r5=1.53216661
a5=89.83996697
d5=117.82833839
r6=1.46984512
a6=89.66937434
d6=-4.56764268
r7=1.53216696
a7=34.27184722
d7=-12.14823188
r8=1.09855456
a8=94.43336109
d8=-132.02735947
r9=1.1140603
a9=95.71409673
d9=96.82000343
r10=1.09669851
a10=110.27705266
d10=-92.82857861
r11=2.04856539
a11=115.63811292
d11=-138.45385344
r12=1.09669853
a12=110.27692191
d12=120.48794562
r13=1.11406079
a13=104.13870186
d13=-125.79450645
r14=1.09464297
a14=143.69890194
d14=-6.29296722
r15=1.09669971
a15=147.42273334
d15=-135.40795704
r16=1.09342186

a16=111.32996713
d16=148.94931642
r17=1.1097952
a17=43.92300133
d17=-106.03926321
r18=1.09342165
a18=111.33002517
d18=-121.29021544
r19=1.09402717
a19=106.20402016
d19=120.18018714
r20=1.09402743
a20=106.2039571
d20=-120.17989026

1-methyl-cyclohexyl cation **6A**

E (MP2/6-31G(d)) = -273.2812865 Hartree

E (MP2/6-31G(d)) + ZPE = -273.0929835 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
C,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,3,R7,2,A7,1,D7,0
H,4,R8,2,A8,6,D8,0
C,3,R9,7,A9,2,D9,0
H,4,R10,2,A10,6,D10,0
C,6,R11,4,A11,2,D11,0
H,6,R12,4,A12,11,D12,0
H,7,R13,3,A13,2,D13,0
H,9,R14,3,A14,2,D14,0
H,6,R15,4,A15,11,D15,0
H,7,R16,3,A16,13,D16,0
H,9,R17,3,A17,14,D17,0
H,9,R18,3,A18,14,D18,0
H,11,R19,6,A19,4,D19,0
H,11,R20,6,A20,19,D20,0
Variables:
R2=1.09637563
R3=1.46290586
R4=1.53547104
R5=1.11431828
R6=1.52529528
R7=1.46290573
R8=1.09556058
R9=1.46264623
R10=1.09329897
R11=1.52529592
R12=1.09762396
R13=1.11431799
R14=1.10817158
R15=1.09396139
R16=1.09637465
R17=1.09218393
R18=1.09218297
R19=1.09555978
R20=1.09329835
A3=110.86941342
A4=114.2130349
A5=104.37656328
A6=111.40370129
A7=120.32135662
A8=108.62311237
A9=119.81166264
A10=108.41835985
A11=110.55846372
A12=110.14715404
A13=100.50579577
A14=103.40415885
A15=109.6540088
A16=110.86967195
A17=113.27299725
A18=113.27347412
A19=110.11205004
A20=111.36975547
D4=-133.38646314

D5=107.4074042
D6=173.33274445
D7=-161.44688255
D8=-121.45444421
D9=177.29641035
D10=122.89067232
D11=-56.84555647
D12=121.96737442
D13=-88.61627974
D14=-91.34748443
D15=-121.02350499
D16=-109.93560503
D17=-115.2010461
D18=115.20191739
D19=-63.73759613
D20=-118.23209997

1-methyl-cyclohexyl cation **6B**

E (B3LYP/6-31G(d)) = -274.3023439 Hartree

E (B3LYP/6-31G(d)) + ZPE = -274.1162919 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,6,R9,2,A9,1,D9,0
H,6,R10,2,A10,9,D10,0
H,6,R11,2,A11,9,D11,0
H,7,R12,2,A12,8,D12,0
H,7,R13,2,A13,8,D13,0
C,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,6,A17,2,D17,0
H,9,R18,6,A18,17,D18,0
H,14,R19,8,A19,7,D19,0
H,14,R20,8,A20,19,D20,0
Variables:
R2=1.46989934
R3=1.09392035
R4=1.10873312
R5=1.09394143
R6=1.45905969
R7=1.45922689
R8=1.60476721
R9=1.60507068
R10=1.09202212
R11=1.09443341
R12=1.09204051
R13=1.09446786
R14=1.5276624
R15=1.09551474
R16=1.09397762
R17=1.09399303
R18=1.0955161
R19=1.09732623
R20=1.09685928
A3=113.42287754
A4=104.76017373
A5=113.4148822
A6=121.00861985
A7=121.00640212
A8=103.29296681
A9=103.23959645
A10=113.63198539
A11=112.20255649
A12=113.61734207
A13=112.1717583
A14=110.53699694
A15=109.03445132
A16=105.48700726
A17=105.46426991
A18=109.04152606
A19=109.03271402
A20=110.17263913
D4=-115.33254354
D5=129.35507018
D6=20.72609553

D7=-170.97364463
D8=102.85511349
D9=-102.82330595
D10=118.60310855
D11=-114.61967161
D12=-118.6354006
D13=114.64735426
D14=56.34496482
D15=-122.6716762
D16=122.15508193
D17=-178.59709594
D18=-115.16127251
D19=-175.6707955
D20=-116.79043517

1-methyl-cyclohexyl cation **6B**

E (MP2/6-31G(d)) = -273.2861339 Hartree

E (MP2/6-31G(d)) + ZPE = -273.0978309 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,6,R9,2,A9,1,D9,0
H,6,R10,2,A10,9,D10,0
H,6,R11,2,A11,9,D11,0
H,7,R12,2,A12,8,D12,0
H,7,R13,2,A13,8,D13,0
C,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,6,A17,2,D17,0
H,9,R18,6,A18,17,D18,0
H,14,R19,8,A19,7,D19,0
H,14,R20,8,A20,19,D20,0
Variables:
R2=1.46729403
R3=1.09227879
R4=1.10645214
R5=1.0922785
R6=1.44880394
R7=1.44883108
R8=1.59904976
R9=1.59909572
R10=1.09170593
R11=1.09248299
R12=1.09170832
R13=1.09248466
R14=1.52010874
R15=1.09514644
R16=1.09389268
R17=1.09389376
R18=1.09514658
R19=1.09629916
R20=1.09577864
A3=113.18923529
A4=104.09936025
A5=113.18903964
A6=120.69038789
A7=120.6892243
A8=100.87371028
A9=100.86676651
A10=113.87991883
A11=113.0687775
A12=113.87671368
A13=113.06591435
A14=110.15192921
A15=109.4182852
A16=105.27586372
A17=105.27167536
A18=109.41880448
A19=109.25230585
A20=110.19880158
D4=-115.54262666
D5=128.91471876

D6=20.62167312
D7=-170.16837266
D8=98.20822751
D9=-98.20896854
D10=117.11508052
D11=-114.24084662
D12=-117.11937069
D13=114.24502119
D14=57.73461582
D15=-122.6950668
D16=121.95353745
D17=-179.69261265
D18=-115.34942509
D19=-177.37108166
D20=-117.14291406

1,4-dimethyl-cyclohexyl cation **7A**

E (B3LYP/6-31G(d)) = -313.6161671 Hartree

E (B3LYP/6-31G(d)) + ZPE = -313.4036861 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,3,R7,1,A7,2,D7,0
C,2,R8,1,A8,6,D8,0
H,2,R9,1,A9,6,D9,0
H,3,R10,1,A10,7,D10,0
H,3,R11,1,A11,7,D11,0
C,6,R12,2,A12,1,D12,0
C,7,R13,3,A13,1,D13,0
H,6,R14,2,A14,12,D14,0
H,6,R15,2,A15,12,D15,0
H,8,R16,2,A16,1,D16,0
H,8,R17,2,A17,16,D17,0
H,8,R18,2,A18,16,D18,0
H,12,R19,6,A19,2,D19,0
H,12,R20,6,A20,19,D20,0
H,13,R21,7,A21,3,D21,0
H,13,R22,7,A22,21,D22,0
H,13,R23,7,A23,21,D23,0
Variables:
R2=1.53667009
R3=1.54536884
R4=1.09406117
R5=1.0976313
R6=1.53667027
R7=1.4686718
R8=1.53410444
R9=1.1012589
R10=1.11428843
R11=1.09690731
R12=1.545369
R13=1.46766894
R14=1.09763109
R15=1.09406116
R16=1.09647351
R17=1.09467607
R18=1.09467605
R19=1.09690598
R20=1.11428797
R21=1.09398347
R22=1.09398677
R23=1.10964071
A3=112.66352167
A4=110.93624557
A5=109.89442433
A6=109.65163844
A7=116.17160326
A8=111.28108186
A9=108.19905001
A10=108.93773704
A11=113.96803275
A12=112.66323659
A13=120.05334623
A14=109.8945258
A15=110.93627623
A16=111.19723581
A17=110.94034465
A18=110.94033344

A19=113.96828023
A20=108.93737353
A21=113.45098765
A22=113.44960165
A23=104.40584705
D4=-121.46518661
D5=120.93999043
D6=-54.94804998
D7=42.42482537
D8=-123.55142385
D9=117.8073236
D10=-113.47710486
D11=130.88127538
D12=54.94888666
D13=152.56824442
D14=-120.94003198
D15=121.46501388
D16=61.30941981
D17=-120.12303004
D18=120.12302799
D19=-173.30777352
D20=-115.64181207
D21=24.15052724
D22=129.59396624
D23=-115.2041446

1,4-dimethyl-cyclohexyl cation **7A**

E (MP2/6-31G(d)) = -312.4515095 Hartree

E (MP2/6-31G(d)) + ZPE = -312.2346215 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,3,R7,1,A7,2,D7,0
C,2,R8,1,A8,6,D8,0
H,2,R9,1,A9,6,D9,0
H,3,R10,1,A10,7,D10,0
H,3,R11,1,A11,7,D11,0
C,6,R12,2,A12,1,D12,0
C,7,R13,3,A13,1,D13,0
H,6,R14,2,A14,12,D14,0
H,6,R15,2,A15,12,D15,0
H,8,R16,2,A16,1,D16,0
H,8,R17,2,A17,16,D17,0
H,8,R18,2,A18,16,D18,0
H,12,R19,6,A19,2,D19,0
H,12,R20,6,A20,19,D20,0
H,13,R21,7,A21,3,D21,0
H,13,R22,7,A22,21,D22,0
H,13,R23,7,A23,21,D23,0
Variables:
R2=1.52763017
R3=1.53432963
R4=1.09424803
R5=1.09683863
R6=1.52763016
R7=1.46198276
R8=1.52635539
R9=1.10077694
R10=1.11453451
R11=1.09673055
R12=1.53432967
R13=1.46285082
R14=1.09683863
R15=1.09424803
R16=1.09465026
R17=1.09326199
R18=1.09326199
R19=1.09673057
R20=1.11453451
R21=1.09217193
R22=1.09217164
R23=1.10804037
A3=112.26582526
A4=110.92687247
A5=109.57884033
A6=109.33667181
A7=116.03154083
A8=111.07221551
A9=108.44062522
A10=109.31763037
A11=114.29809187
A12=112.265852
A13=119.89635472
A14=109.57883209
A15=110.92687047
A16=110.6852291
A17=110.88977438

A18=110.88977622
A19=114.29807532
A20=109.31766733
A21=113.27378289
A22=113.27388498
A23=103.41475955
D4=-121.47013917
D5=121.00420662
D6=-56.47819169
D7=42.60190814
D8=-122.92608939
D9=118.05946589
D10=-112.63185891
D11=130.9871259
D12=56.47812761
D13=154.24873109
D14=-121.00419609
D15=121.4701597
D16=60.96024519
D17=-120.03460762
D18=120.03460808
D19=-173.58887502
D20=-116.3810069
D21=23.83839828
D22=129.57623178
D23=-115.21175526

1,4-dimethyl-cyclohexyl cation **7B**

E (B3LYP/6-31G(d)) = -313.6179664 Hartree

E (B3LYP/6-31G(d)) + ZPE = -313.4054869 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,6,R9,2,A9,1,D9,0
H,6,R10,2,A10,9,D10,0
H,6,R11,2,A11,9,D11,0
H,7,R12,2,A12,8,D12,0
H,7,R13,2,A13,8,D13,0
C,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,6,A17,2,D17,0
H,9,R18,6,A18,17,D18,0
C,14,R19,8,A19,7,D19,0
H,14,R20,8,A20,19,D20,0
H,19,R21,14,A21,8,D21,0
H,19,R22,14,A22,21,D22,0
H,19,R23,14,A23,21,D23,0
Variables:
R2=1.46934013
R3=1.0938934
R4=1.10904433
R5=1.09391068
R6=1.45992681
R7=1.45994025
R8=1.60118558
R9=1.60122499
R10=1.09211944
R11=1.09482858
R12=1.09211945
R13=1.09482117
R14=1.53170057
R15=1.09658486
R16=1.09440618
R17=1.09438986
R18=1.09659497
R19=1.5411223
R20=1.0992893
R21=1.09603803
R22=1.09398516
R23=1.09400731
A3=113.46385912
A4=104.68981891
A5=113.4582899
A6=121.05395689
A7=121.04885452
A8=103.44929511
A9=103.46848671
A10=113.51139009
A11=112.0129177
A12=113.51240759
A13=112.01996327
A14=111.42413876
A15=109.18259926
A16=105.38925927
A17=105.38563207

A18=109.18118018
A19=110.92678793
A20=108.29517703
A21=111.32139551
A22=110.7114268
A23=110.72733911
D4=-115.26394411
D5=129.48747344
D6=20.84332651
D7=-171.2230257
D8=104.0406945
D9=-104.05282406
D10=118.99334484
D11=-114.74273127
D12=-118.98481298
D13=114.74559919
D14=56.77774431
D15=-122.78447934
D16=122.22160004
D17=-178.9541
D18=-114.99480756
D19=-178.36192657
D20=-118.57775034
D21=60.80323169
D22=-120.26192106
D23=120.26254527

1,4-dimethyl-cyclohexyl cation **7B**

E (MP2/6-31G(d)) = -312.4559264 Hartree

E (MP2/6-31G(d)) + ZPE = -312.2365338 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,6,R9,2,A9,1,D9,0
H,6,R10,2,A10,9,D10,0
H,6,R11,2,A11,9,D11,0
H,7,R12,2,A12,8,D12,0
H,7,R13,2,A13,8,D13,0
C,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,6,A17,2,D17,0
H,9,R18,6,A18,17,D18,0
C,14,R19,8,A19,7,D19,0
H,14,R20,8,A20,19,D20,0
H,19,R21,14,A21,8,D21,0
H,19,R22,14,A22,21,D22,0
H,19,R23,14,A23,21,D23,0
Variables:
R2=1.46707977
R3=1.0922474
R4=1.10658983
R5=1.09224862
R6=1.44869473
R7=1.44868393
R8=1.59692584
R9=1.59691302
R10=1.09181273
R11=1.09252902
R12=1.09181071
R13=1.09252322
R14=1.52322458
R15=1.09657419
R16=1.09461903
R17=1.09460699
R18=1.09658306
R19=1.53208957
R20=1.09868425
R21=1.0943368
R22=1.0926656
R23=1.09268023
A3=113.18543417
A4=104.04579313
A5=113.18538443
A6=120.71599197
A7=120.71574385
A8=100.6962872
A9=100.71274898
A10=113.85790689
A11=113.06236411
A12=113.8598396
A13=113.06795584
A14=111.11021015
A15=109.60686225
A16=105.30142189
A17=105.30051561
A18=109.6086837

A19=110.83227132
A20=108.41488967
A21=110.86747866
A22=110.71411929
A23=110.72551947
D4=-115.52639982
D5=128.9485128
D6=20.63476541
D7=-170.21554039
D8=98.40995884
D9=-98.41752677
D10=117.14392214
D11=-114.28298628
D12=-117.13549173
D13=114.28220725
D14=58.03190306
D15=-122.72210221
D16=121.98599479
D17=-179.98395943
D18=-115.29478535
D19=-179.09061974
D20=-118.99668549
D21=60.63038764
D22=-120.20313398
D23=120.20474473

1,3,3-trimethyl-cyclohexyl cation **8**

E (B3LYP/6-31G(d)) = -156.2964481 Hartree

E (B3LYP/6-31G(d)) + ZPE = -156.0560031 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,3,R7,1,A7,2,D7,0
H,2,R8,1,A8,6,D8,0
H,2,R9,1,A9,6,D9,0
H,3,R10,1,A10,7,D10,0
H,3,R11,1,A11,7,D11,0
C,6,R12,2,A12,1,D12,0
C,7,R13,3,A13,1,D13,0
C,6,R14,2,A14,12,D14,0
C,6,R15,2,A15,12,D15,0
H,12,R16,6,A16,2,D16,0
H,12,R17,6,A17,16,D17,0
H,13,R18,7,A18,3,D18,0
H,13,R19,7,A19,18,D19,0
H,13,R20,7,A20,18,D20,0
H,14,R21,6,A21,2,D21,0
H,14,R22,6,A22,21,D22,0
H,14,R23,6,A23,21,D23,0
H,15,R24,6,A24,2,D24,0
H,15,R25,6,A25,24,D25,0
H,15,R26,6,A26,24,D26,0
Variables:
R2=1.53825856
R3=1.5340295
R4=1.09343404
R5=1.09712739
R6=1.55299107
R7=1.47307122
R8=1.09437549
R9=1.09820847
R10=1.10213481
R11=1.10896502
R12=1.62339176
R13=1.47054931
R14=1.53663887
R15=1.53809494
R16=1.0916917
R17=1.10318122
R18=1.10651921
R19=1.09746098
R20=1.09199014
R21=1.09562502
R22=1.09526481
R23=1.09679487
R24=1.09609057
R25=1.09534268
R26=1.09516872
A3=108.93712223
A4=110.98341
A5=110.73330196
A6=113.33801537
A7=113.74281883
A8=109.94899805
A9=108.15292575
A10=113.05339749
A11=112.30744704
A12=109.77074482

A13=120.96630621
A14=111.1916942
A15=111.34178814
A16=111.08681435
A17=103.74248201
A18=106.56000464
A19=111.33444276
A20=113.95418098
A21=109.45136426
A22=111.71426515
A23=112.30253898
A24=111.83348362
A25=111.61679359
A26=109.46844705
D4=-120.28630547
D5=121.78310166
D6=-61.53666127
D7=44.21111649
D8=-122.51388356
D9=121.67632957
D10=-124.27644016
D11=119.7191984
D12=21.36209891
D13=-164.26689779
D14=119.36481815
D15=-117.29676877
D16=164.08574533
D17=117.18923542
D18=107.80424585
D19=113.64606171
D20=-119.45336243
D21=59.76020644
D22=118.93129125
D23=-118.96857924
D24=51.96531795
D25=121.44475096
D26=-119.43042614

1,3,3-trimethyl-cyclohexyl **8**

E (MP2/6-31G(d)) = -351.6220254 Hartree
E (MP2/6-31G(d)) + ZPE = -351.3766324 Hartree
NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,3,R7,1,A7,2,D7,0
C,2,R8,1,A8,6,D8,0
C,2,R9,1,A9,6,D9,0
H,3,R10,1,A10,7,D10,0
H,3,R11,1,A11,7,D11,0
C,6,R12,2,A12,1,D12,0
C,7,R13,3,A13,1,D13,0
H,6,R14,2,A14,12,D14,0
H,6,R15,2,A15,12,D15,0
H,8,R16,2,A16,1,D16,0
H,8,R17,2,A17,16,D17,0
H,8,R18,2,A18,16,D18,0
H,9,R19,2,A19,1,D19,0
H,9,R20,2,A20,19,D20,0
H,9,R21,2,A21,19,D21,0
H,12,R22,6,A22,2,D22,0
H,12,R23,6,A23,22,D23,0
H,13,R24,7,A24,3,D24,0
H,13,R25,7,A25,24,D25,0
H,13,R26,7,A26,24,D26,0
Variables:
R2=1.53312708
R3=1.53548951
R4=1.09684178
R5=1.0951911
R6=1.53312705
R7=1.4601062
R8=1.53053708
R9=1.53190532
R10=1.09676641
R11=1.1141204
R12=1.53548956
R13=1.46357671
R14=1.0951911
R15=1.09684177
R16=1.09428548
R17=1.09428548
R18=1.09477735
R19=1.09671296
R20=1.09431931
R21=1.09431931
R22=1.09676641
R23=1.1141204
R24=1.10774418
R25=1.09220106
R26=1.09220104
A3=113.22515861
A4=109.63119174
A5=110.49639616
A6=108.15795092
A7=115.93963147
A8=108.83179514

A9=111.00424554
A10=113.9675554
A11=109.69936355
A12=113.22515879
A13=120.05525766
A14=110.49639519
A15=109.63119251
A16=110.61924627
A17=110.61924752
A18=111.20352391
A19=113.69065283
A20=110.35227946
A21=110.35227442
A22=113.96755574
A23=109.69935943
A24=103.55712267
A25=113.22138721
A26=113.22138667
D4=-120.99342279
D5=121.7993511
D6=55.53503849
D7=-43.16456866
D8=118.08457025
D9=-122.0051412
D10=-130.66020282
D11=113.01920472
D12=-55.53503614
D13=-153.2149053
D14=-121.79934503
D15=120.99342617
D16=61.3982418
D17=119.54513998
D18=-120.22743026
D19=60.16546022
D20=120.56827763
D21=-120.5682748
D22=173.82476879
D23=116.32059171
D24=91.2981828
D25=115.29654229
D26=-115.29654141

cyclopentyl cation **9**

E (B3LYP/6-31G(d)) = -195.6368124 Hartree

E (B3LYP/6-31G(d)) + ZPE = -195.5107494 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,r2
C,2,r3,1,a3
C,3,r4,2,a4,1,d4,0
C,4,r5,3,a5,2,d5,0
C,2,r6,1,a6,3,d6,0
H,2,r7,1,a7,3,d7,0
H,6,r8,2,a8,1,d8,0
H,3,r9,2,a9,1,d9,0
H,4,r10,3,a10,2,d10,0
H,4,r11,3,a11,2,d11,0
H,5,r12,4,a12,3,d12,0
H,5,r13,4,a13,3,d13,0
H,6,r14,2,a14,1,d14,0
Variables:
r2=1.096899
r3=1.44621723
a3=115.93364158
r4=1.446293
a4=111.82283111
d4=146.33832382
r5=1.54858001
a5=105.94119865
d5=9.97031101
r6=1.54852856
a6=120.33390678
d6=129.67045466
r7=1.12469562
a7=103.6778565
d7=-107.28797922
r8=1.09102588
a8=112.19235732
d8=78.00394036
r9=1.09185269
a9=124.08742741
d9=-33.71525888
r10=1.09690241
a10=115.93524732
d10=146.25678384
r11=1.12461917
a11=98.99279687
d11=-103.66495027
r12=1.0910289
a12=112.19319791
d12=-148.00463695
r13=1.09559335
a13=108.93395512
d13=92.73839834
r14=1.09559755
a14=108.93437687
d14=-41.2534722

cyclopentyl cation **9**

E (MP2/6-31G(d)) = -194.9141583 Hartree

E (MP2/6-31G(d)) + ZPE = -194.7854573 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,3,R7,1,A7,2,D7,0
H,2,R8,1,A8,6,D8,0
H,2,R9,1,A9,6,D9,0
H,3,R10,1,A10,7,D10,0
H,3,R11,1,A11,7,D11,0
H,6,R12,2,A12,1,D12,0
H,7,R13,3,A13,1,D13,0
H,7,R14,3,A14,13,D14,0
Variables:
R2=1.5406838
R3=1.55503403
R4=1.09112789
R5=1.09112904
R6=1.43981599
R7=1.54068353
R8=1.1091754
R9=1.1091743
R10=1.09112859
R11=1.09112827
R12=1.09236919
R13=1.10916004
R14=1.10919019
A3=106.12647112
A4=110.39401661
A5=110.39194023
A6=107.02493407
A7=106.12642985
A8=116.35863805
A9=116.35941116
A10=111.38441925
A11=111.38463086
A12=123.15137605
A13=116.36302366
A14=116.35515537
D4=-120.82688616
D5=120.8245417
D6=-0.00808189
D7=0.00273231
D8=-120.47938137
D9=120.48295649
D10=-120.18307879
D11=120.18368486
D12=-179.99463814
D13=120.49909474
D14=119.0376428

1-cyclopropyl-isopropyl cation **10**

E (B3LYP/6-31G(d)) = -156.2964481 Hartree

E (B3LYP/6-31G(d)) + ZPE = -156.1375667 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,r2
C,2,r3,1,a3
C,3,r4,2,a4,1,d4,0
H,4,r5,3,a5,2,d5,0
H,4,r6,3,a6,2,d6,0
H,1,r7,2,a7,3,d7,0
H,1,r8,2,a8,3,d8,0
H,2,r9,1,a9,3,d9,0
H,2,r10,1,a10,3,d10,0
H,3,r11,2,a11,1,d11,0
Variables:
r2=1.42031367
r3=1.63728612
a3=66.26423626
r4=1.3590873
a4=118.99201238
d4=-100.46027204
r5=1.0888385
a5=121.16124813
d5=-155.58457767
r6=1.08869016
a6=122.02993275
d6=24.41769704
r7=1.08727946
a7=120.95184575
d7=-93.90025129
r8=1.08522833
a8=120.86483706
d8=102.50429411
r9=1.08547558
a9=120.26737076
d9=-104.38958868
r10=1.08743654
a10=120.24383669
d10=97.27477093
r11=1.08388048
a11=115.31149017
d11=101.9174551

1-cyclopropyl-isopropyl cation **10**

E (MP2/6-31G(d)) = 155.7257500 Hartree

E (MP2/6-31G(d)) + ZPE = -155.5743332 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,3,D7,0
H,2,R8,1,A8,7,D8,0
H,3,R9,1,A9,6,D9,0
H,6,R10,3,A10,1,D10,0
H,6,R11,3,A11,10,D11,0
Variables:
R2=1.41634038
R3=1.64815198
R4=1.08644143
R5=1.08465345
R6=1.35734814
R7=1.08465229
R8=1.08644471
R9=1.08331315
R10=1.08776368
R11=1.08825628
A3=64.55212624
A4=120.53422607
A5=120.50229298
A6=116.43907273
A7=120.50334572
A8=120.53365734
A9=115.25339139
A10=121.19148203
A11=121.71862559
D4=-95.47644898
D5=102.96449167
D6=103.68643839
D7=-102.96714625
D8=-161.55373327
D9=153.34008757
D10=151.32272936
D11=179.99949069

1-cyclopropyl-isopropyl cation **10**

E (MP2/6-31G(d)) = 155.7257500 Hartree

E (MP2/6-31G(d)) + ZPE = -155.5743332 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,3,D7,0
H,2,R8,1,A8,7,D8,0
H,3,R9,1,A9,6,D9,0
H,6,R10,3,A10,1,D10,0
H,6,R11,3,A11,10,D11,0
Variables:
R2=1.41634038
R3=1.64815198
R4=1.08644143
R5=1.08465345
R6=1.35734814
R7=1.08465229
R8=1.08644471
R9=1.08331315
R10=1.08776368
R11=1.08825628
A3=64.55212624
A4=120.53422607
A5=120.50229298
A6=116.43907273
A7=120.50334572
A8=120.53365734
A9=115.25339139
A10=121.19148203
A11=121.71862559
D4=-95.47644898
D5=102.96449167
D6=103.68643839
D7=-102.96714625
D8=-161.55373327
D9=153.34008757
D10=151.32272936
D11=179.99949069

3-methyl-3-pentyl cation **11**

E (B3LYP/6-31G(d)) = -236.1885249 Hartree

E (B3LYP/6-31G(d)) + ZPE = -236.0117139 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,r2
C,2,r3,1,a3
C,2,r4,1,a4,3,d4,0
H,3,r5,2,a5,1,d5,0
H,1,r6,2,a6,3,d6,0
H,1,r7,2,a7,3,d7,0
C,1,r8,2,a8,3,d8,0
H,4,r9,2,a9,1,d9,0
C,4,r10,2,a10,1,d10,0
H,4,r11,2,a11,1,d11,0
H,8,r12,1,a12,2,d12,0
H,8,r13,1,a13,2,d13,0
H,8,r14,1,a14,2,d14,0
H,10,r15,4,a15,2,d15,0
H,10,r16,4,a16,2,d16,0
H,10,r17,4,a17,2,d17,0
H,3,r18,2,a18,1,d18,0
H,3,r19,2,a19,1,d19,0
Variables:
r2=1.46484129
r3=1.47238753
a3=119.48083782
r4=1.46534642
a4=120.08668158
d4=-178.52353019
r5=1.09647265
a5=111.72597873
d5=33.70229097
r6=1.09464744
a6=111.47424843
d6=150.32051602
r7=1.09390341
a7=112.24137935
d7=25.55267519
r8=1.58088086
a8=105.96732933
d8=-92.5831125
r9=1.09451712
a9=111.61842573
d9=-143.93991643
r10=1.58070432
a10=106.61802934
d10=98.52481605
r11=1.09352145
a11=111.72084932
d11=-19.66943373
r12=1.09228531
a12=111.71287015
d12=-61.25850722
r13=1.09299023
a13=106.32819027
d13=-179.77566217
r14=1.09237187
a14=111.62459402
d14=61.79289321
r15=1.09282507
a15=106.44310496
d15=-177.43878475
r16=1.09207441
a16=111.47818255
d16=64.02526068
r17=1.09275667

a17=111.64254618
d17=-59.05945376
r18=1.10663956
a18=106.21396302
d18=-79.86982598
r19=1.09161942
a19=114.08405253
d19=161.15573367

3-methyl-3-pentyl cation **11**

E (MP2/6-31G(d)) = -235.2807201 Hartree

E (MP2/6-31G(d)) + ZPE = -235.1003041 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
H,5,R8,1,A8,2,D8,0
H,5,R9,1,A9,8,D9,0
H,5,R10,1,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,7,R12,2,A12,1,D12,0
C,7,R13,2,A13,12,D13,0
H,7,R14,2,A14,12,D14,0
H,6,R15,2,A15,11,D15,0
H,6,R16,2,A16,11,D16,0
H,13,R17,7,A17,2,D17,0
H,13,R18,7,A18,17,D18,0
H,13,R19,7,A19,17,D19,0
Variables:
R2=1.45550011
R3=1.09302906
R4=1.09244836
R5=1.57418169
R6=1.46843562
R7=1.45588933
R8=1.09088509
R9=1.09164806
R10=1.09087371
R11=1.09460508
R12=1.09270076
R13=1.57410963
R14=1.09206011
R15=1.10441613
R16=1.09006197
R17=1.09141109
R18=1.09043609
R19=1.09160398
A3=112.00582975
A4=112.73734141
A5=103.52522975
A6=119.49912314
A7=120.0451235
A8=111.6707494
A9=106.21509022
A10=111.71703727
A11=111.35539143
A12=112.25925872
A13=104.01781423
A14=112.17534475
A15=105.75096212
A16=113.76199318
A17=106.36649913
A18=111.32828279
A19=111.74144609
D4=-126.08471437
D5=116.41751886
D6=151.20918326
D7=-178.00050287
D8=-61.51979092
D9=-118.3764561
D10=123.31476862
D11=34.18426894
D12=-144.6592658

D13=-116.89320827
D14=125.65476367
D15=-113.80002202
D16=126.99638132
D17=-175.09446704
D18=-118.44481483
D19=118.27359744
Final structure in terms of initial Z-matrix:
C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
C,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
H,5,R8,1,A8,2,D8,0
H,5,R9,1,A9,8,D9,0
H,5,R10,1,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,7,R12,2,A12,1,D12,0
C,7,R13,2,A13,12,D13,0
H,7,R14,2,A14,12,D14,0
H,6,R15,2,A15,11,D15,0
H,6,R16,2,A16,11,D16,0
H,13,R17,7,A17,2,D17,0
H,13,R18,7,A18,17,D18,0
H,13,R19,7,A19,17,D19,0
Variables:
R2=1.45550011
R3=1.09302906
R4=1.09244836
R5=1.57418169
R6=1.46843562
R7=1.45588933
R8=1.09088509
R9=1.09164806
R10=1.09087371
R11=1.09460508
R12=1.09270076
R13=1.57410963
R14=1.09206011
R15=1.10441613
R16=1.09006197
R17=1.09141109
R18=1.09043609
R19=1.09160398
A3=112.00582975
A4=112.73734141
A5=103.52522975
A6=119.49912314
A7=120.0451235
A8=111.6707494
A9=106.21509022
A10=111.71703727
A11=111.35539143
A12=112.25925872
A13=104.01781423
A14=112.17534475
A15=105.75096212
A16=113.76199318
A17=106.36649913
A18=111.32828279
A19=111.74144609
D4=-126.08471437
D5=116.41751886
D6=151.20918326
D7=-178.00050287
D8=-61.51979092
D9=-118.3764561
D10=123.31476862
D11=34.18426894
D12=-144.6592658
D13=-116.89320827
D14=125.65476367

D15=-113.80002202
D16=126.99638132
D17=-175.09446704
D18=-118.44481483
D19=118.27359744

2,4-dimetyl-2-pentyl cation **12**

E (B3LYP/6-31G(d)) = -275.5043225 Hartree

E (B3LYP/6-31G(d)) + ZPE = -275.3003235 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
H,7,R9,2,A9,8,D9,0
H,7,R10,2,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,6,R12,2,A12,11,D12,0
H,6,R13,2,A13,11,D13,0
C,8,R14,7,A14,2,D14,0
C,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,14,R17,8,A17,7,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
H,15,R20,8,A20,7,D20,0
H,15,R21,8,A21,20,D21,0
H,15,R22,8,A22,20,D22,0
Variables:
R2=1.47164939
R3=1.09495106
R4=1.10795607
R5=1.09271546
R6=1.47291037
R7=1.44916365
R8=1.62743646
R9=1.0949221
R10=1.09319388
R11=1.09061426
R12=1.10397252
R13=1.10024978
R14=1.53300996
R15=1.52940405
R16=1.09593459
R17=1.09561774
R18=1.0941631
R19=1.09529908
R20=1.09486142
R21=1.09661327
R22=1.09570734
A3=112.34938923
A4=105.27655528
A5=114.0296363
A6=118.8930817
A7=120.52845475
A8=109.22439847
A9=110.7567327
A10=112.81306845
A11=114.15781127
A12=108.06066811
A13=109.93329872
A14=106.49942788
A15=112.37888891
A16=106.45360585
A17=108.69493678
A18=112.11155737
A19=111.51081603
A20=109.07884256

A21=111.56662182
A22=113.21072963
D4=114.01010287
D5=-128.64781169
D6=147.890249
D7=-178.76361491
D8=102.18401656
D9=115.25643917
D10=-119.3242738
D11=171.95255217
D12=122.14417274
D13=-124.80966872
D14=173.67237814
D15=123.29578331
D16=-116.36169275
D17=-177.59866468
D18=119.21207573
D19=-118.72361658
D20=-174.95187421
D21=118.16659693
D22=-119.03669863

2,4-dimethyl-2-pentyl cation **12**

E (MP2/6-31G(d)) = -274.4500894 Hartree

E (MP2/6-31G(d)) + ZPE = -274.26566464

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
H,7,R9,2,A9,8,D9,0
H,7,R10,2,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,6,R12,2,A12,11,D12,0
H,6,R13,2,A13,11,D13,0
C,8,R14,7,A14,2,D14,0
C,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,14,R17,8,A17,7,D17,0
H,14,R18,8,A18,17,D18,0
H,14,R19,8,A19,17,D19,0
H,15,R20,8,A20,7,D20,0
H,15,R21,8,A21,20,D21,0
H,15,R22,8,A22,20,D22,0
Variables:
R2=1.46532815
R3=1.09159163
R4=1.107483
R5=1.09187468
R6=1.46864465
R7=1.43912973
R8=1.61251064
R9=1.09349634
R10=1.09230883
R11=1.08934124
R12=1.10281952
R13=1.09723288
R14=1.52772469
R15=1.52420369
R16=1.09546351
R17=1.09382385
R18=1.09265138
R19=1.09350708
R20=1.09308082
R21=1.09489732
R22=1.09435253
A3=112.82410901
A4=103.72757346
A5=113.7020581
A6=118.796669
A7=120.69869442
A8=105.64240619
A9=111.93830118
A10=113.43485338
A11=113.75481603
A12=107.08668959
A13=110.11961649
A14=106.09149278
A15=112.75997884
A16=106.80128622
A17=108.74044407
A18=111.92852107
A19=110.96851872
A20=108.9609551
A21=111.05974557

A22=113.38718421
D4=114.55049839
D5=-129.35384622
D6=152.81069866
D7=-178.03750217
D8=102.08388279
D9=114.49197984
D10=-117.90842831
D11=168.61026966
D12=121.14510507
D13=-125.2944021
D14=177.72103183
D15=122.60409052
D16=-116.38470173
D17=-176.9968342
D18=119.4060272
D19=-118.7619553
D20=-173.76827388
D21=118.11501856
D22=-119.19280899

2,3-dimethyl-2-butyl cation **13**

E (B3LYP/6-31G(d)) = -236.1885221 Hartree

E (B3LYP/6-31G(d)) + ZPE = -236.0130191 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,4,R7,2,A7,6,D7,0
H,7,R8,4,A8,2,D8,0
H,7,R9,4,A9,8,D9,0
H,7,R10,4,A10,8,D10,0
H,6,R11,4,A11,2,D11,0
C,6,R12,4,A12,11,D12,0
C,6,R13,4,A13,11,D13,0
H,13,R14,6,A14,4,D14,0
H,12,R15,6,A15,4,D15,0
H,12,R16,6,A16,15,D16,0
H,12,R17,6,A17,15,D17,0
H,13,R18,6,A18,14,D18,0
H,13,R19,6,A19,14,D19,0
Variables:
R2=1.08343633
R3=1.07985387
R4=1.4758045
R5=1.09412545
R6=1.47603607
R7=1.47680286
R8=1.09274519
R9=1.08276654
R10=1.07981324
R11=1.08446274
R12=1.56955663
R13=1.53182821
R14=1.08403591
R15=1.0827608
R16=1.0828009
R17=1.08203444
R18=1.08241211
R19=1.08295658
A3=111.47661881
A4=111.75476267
A5=106.38546048
A6=119.68162643
A7=118.82419427
A8=105.7195508
A9=111.82234876
A10=113.06375529
A11=108.03247856
A12=103.31790711
A13=116.31402219
A14=111.7246166
A15=112.80991356
A16=111.52608631
A17=106.73587627
A18=108.54813309
A19=112.44342324
D4=-127.97457283
D5=117.8561683
D6=138.23873467
D7=179.45024032
D8=-100.97529108
D9=-115.09817706
D10=118.68732994
D11=25.68840592

D12=-112.96974491
D13=124.50557272
D14=-58.98473433
D15=56.8826732
D16=-123.44320179
D17=118.47454744
D18=-118.41272716
D19=122.65877845

2,3-dimethyl-2-butyl cation **13**

E (B3LYP/6-31G(d)) = -236.1885221 Hartree

E (B3LYP/6-31G(d)) + ZPE = -236.0130191 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,4,R7,2,A7,6,D7,0
H,7,R8,4,A8,2,D8,0
H,7,R9,4,A9,8,D9,0
H,7,R10,4,A10,8,D10,0
H,6,R11,4,A11,2,D11,0
C,6,R12,4,A12,11,D12,0
C,6,R13,4,A13,11,D13,0
H,13,R14,6,A14,4,D14,0
H,12,R15,6,A15,4,D15,0
H,12,R16,6,A16,15,D16,0
H,12,R17,6,A17,15,D17,0
H,13,R18,6,A18,14,D18,0
H,13,R19,6,A19,14,D19,0
Variables:
R2=1.08343633
R3=1.07985387
R4=1.4758045
R5=1.09412545
R6=1.47603607
R7=1.47680286
R8=1.09274519
R9=1.08276654
R10=1.07981324
R11=1.08446274
R12=1.56955663
R13=1.53182821
R14=1.08403591
R15=1.0827608
R16=1.0828009
R17=1.08203444
R18=1.08241211
R19=1.08295658
A3=111.47661881
A4=111.75476267
A5=106.38546048
A6=119.68162643
A7=118.82419427
A8=105.7195508
A9=111.82234876
A10=113.06375529
A11=108.03247856
A12=103.31790711
A13=116.31402219
A14=111.7246166
A15=112.80991356
A16=111.52608631
A17=106.73587627
A18=108.54813309
A19=112.44342324
D4=-127.97457283
D5=117.8561683
D6=138.23873467
D7=179.45024032
D8=-100.97529108
D9=-115.09817706
D10=118.68732994
D11=25.68840592

D12=-112.96974491
D13=124.50557272
D14=-58.98473433
D15=56.8826732
D16=-123.44320179
D17=118.47454744
D18=-118.41272716
D19=122.65877845

2,3-dimethyl-2-butyl cation **13**

E (MP2/6-31G(d)) = -235.282151 Hartree

E (MP2/6-31G(d)) + ZPE = -235.1397889 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

H
C,1,R2
H,2,R3,1,A3
C,2,R4,1,A4,3,D4,0
H,2,R5,1,A5,3,D5,0
C,4,R6,2,A6,1,D6,0
C,4,R7,2,A7,6,D7,0
H,7,R8,4,A8,2,D8,0
H,7,R9,4,A9,8,D9,0
H,7,R10,4,A10,8,D10,0
H,6,R11,4,A11,2,D11,0
C,6,R12,4,A12,11,D12,0
C,6,R13,4,A13,11,D13,0
H,13,R14,6,A14,4,D14,0
H,12,R15,6,A15,4,D15,0
H,12,R16,6,A16,15,D16,0
H,12,R17,6,A17,15,D17,0
H,13,R18,6,A18,14,D18,0
H,13,R19,6,A19,14,D19,0
Variables:
R2=1.10442247
R3=1.08936587
R4=1.46870453
R5=1.09576503
R6=1.44661985
R7=1.46925219
R8=1.09222891
R9=1.1050819
R10=1.09047421
R11=1.09412111
R12=1.5239101
R13=1.59288072
R14=1.09079696
R15=1.09333847
R16=1.0928472
R17=1.09190934
R18=1.09277994
R19=1.09192948
A3=108.64953221
A4=105.65124484
A5=105.26496303
A6=120.09257035
A7=118.71731579
A8=112.63668055
A9=105.02802321
A10=113.38854255
A11=110.13219917
A12=118.47538645
A13=98.31336918
A14=113.21055583
A15=111.1008657
A16=112.31752903
A17=108.76479441
A18=104.32964612
A19=111.27444835
D4=-122.36853287
D5=119.65477611
D6=114.02538741
D7=179.85063686
D8=-146.72423943
D9=-114.26914366
D10=127.63109531

D11=-24.14478352
D12=-130.45799358
D13=110.18481696
D14=-58.82975111
D15=62.05420605
D16=-122.24593168
D17=118.6087885
D18=-117.96548056
D19=124.77635747

2,3,3-trimethyl-2-butyl cation **14**

E (B3LYP/6-31G(d)) = -275.5013985 Hartree

E (B3LYP/6-31G(d)) + ZPE = -275.3037666 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,7,R9,2,A9,8,D9,0
C,7,R10,2,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,6,R12,2,A12,11,D12,0
H,6,R13,2,A13,11,D13,0
H,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,7,A17,2,D17,0
H,9,R18,7,A18,17,D18,0
H,9,R19,7,A19,17,D19,0
H,10,R20,7,A20,2,D20,0
H,10,R21,7,A21,20,D21,0
H,10,R22,7,A22,20,D22,0
Variables:
R2=1.47387398
R3=1.08847482
R4=1.0958448
R5=1.10762956
R6=1.47742119
R7=1.47133331
R8=1.54042064
R9=1.60427557
R10=1.54685882
R11=1.09694429
R12=1.1038707
R13=1.09059278
R14=1.09307684
R15=1.09543024
R16=1.09318767
R17=1.09501217
R18=1.09266365
R19=1.09213589
R20=1.09329207
R21=1.09216999
R22=1.09461745
A3=115.23687232
A4=111.54874833
A5=105.3261204
A6=116.91157511
A7=122.11348831
A8=114.95486397
A9=98.46998044
A10=114.73085063
A11=111.64969637
A12=107.39871184
A13=113.54000264
A14=108.99814596
A15=111.02670714
A16=113.227818
A17=104.23151656
A18=112.6188865
A19=112.6558818
A20=108.40592443
A21=113.57289016

A22=110.80663424
D4=128.3500912
D5=-118.30671085
D6=-168.20056939
D7=179.51654337
D8=161.32922136
D9=115.41143096
D10=-129.67056204
D11=135.15705567
D12=113.79678113
D13=-125.41763553
D14=175.68986801
D15=118.25501602
D16=-119.33302504
D17=-179.0580324
D18=117.36427478
D19=-117.61176643
D20=-175.65487131
D21=119.19982148
D22=-118.11615445

2,3,3-trimethyl-2-butyl cation **14**

E (MP2/6-31G(d)) = -274.4516058 Hartree

E (MP2/6-31G(d)) + ZPE = -274.2437418 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
H,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,2,R6,1,A6,3,D6,0
C,2,R7,1,A7,6,D7,0
C,7,R8,2,A8,1,D8,0
C,7,R9,2,A9,8,D9,0
C,7,R10,2,A10,8,D10,0
H,6,R11,2,A11,1,D11,0
H,6,R12,2,A12,11,D12,0
H,6,R13,2,A13,11,D13,0
H,8,R14,7,A14,2,D14,0
H,8,R15,7,A15,14,D15,0
H,8,R16,7,A16,14,D16,0
H,9,R17,7,A17,2,D17,0
H,9,R18,7,A18,17,D18,0
H,9,R19,7,A19,17,D19,0
H,10,R20,7,A20,2,D20,0
H,10,R21,7,A21,20,D21,0
H,10,R22,7,A22,20,D22,0
Variables:
R2=1.472
R3=1.08629784
R4=1.09381397
R5=1.1052226
R6=1.47580656
R7=1.44988551
R8=1.52945382
R9=1.60307798
R10=1.5328131
R11=1.09209707
R12=1.10309066
R13=1.08991284
R14=1.09274379
R15=1.09475888
R16=1.09084646
R17=1.09429292
R18=1.09170326
R19=1.09209203
R20=1.09252048
R21=1.09039121
R22=1.09344593
A3=115.11124646
A4=111.33771468
A5=104.67540033
A6=116.6518629
A7=122.2649556
A8=115.74642375
A9=95.01102878
A10=116.13760397
A11=112.70755159
A12=105.75756775
A13=113.0374551
A14=108.76570738
A15=110.53181079
A16=113.32326547
A17=102.74475662
A18=113.04393631
A19=112.79744745
A20=108.31430371
A21=113.44268421
A22=110.54451489

D4=128.01085323
D5=-118.37904143
D6=-170.10674658
D7=-179.813065
D8=159.81184728
D9=113.91401034
D10=-132.56441502
D11=141.72852193
D12=114.70166588
D13=-126.34928978
D14=173.47868106
D15=118.08025877
D16=-119.52824099
D17=-179.15413346
D18=116.88594295
D19=-116.94910571
D20=-175.56169534
D21=119.16440418
D22=-118.05726737

Methyl-cyclopropyl cation **15**

E (B3LYP/6-31G(d)) = -156.2964490 Hartree

E (B3LYP/6-31G(d)) + ZPE = -156.198791 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,3,D7,0
H,2,R8,1,A8,7,D8,0
H,3,R9,1,A9,6,D9,0
H,6,R10,3,A10,1,D10,0
H,6,R11,3,A11,10,D11,0
Variables:
R2=1.42000035
R3=1.65910277
R4=1.08728285
R5=1.08614226
R6=1.35916629
R7=1.08479537
R8=1.08801149
R9=1.08422322
R10=1.0881034
R11=1.08856235
A3=64.68102653
A4=120.66648578
A5=120.56737831
A6=117.37556414
A7=120.62664913
A8=120.57543917
A9=114.88212326
A10=122.0466671
A11=121.11626899
D4=-95.57469679
D5=103.37117392
D6=104.15238639
D7=-103.34619911
D8=-161.13708794
D9=153.12176263
D10=-28.8102576
D11=180.

methyl-cyclopropyl cation **15**

E (MP2/6-31G(d)) = -155.7257500 Hartree

E (MP2/6-31G(d)) + ZPE = -155.626001 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
H,1,R4,2,A4,3,D4,0
H,1,R5,2,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
H,2,R7,1,A7,3,D7,0
H,2,R8,1,A8,7,D8,0
H,3,R9,1,A9,6,D9,0
H,6,R10,3,A10,1,D10,0
H,6,R11,3,A11,10,D11,0
Variables:
R2=1.45200034
R3=1.58797859
R4=1.11203957
R5=1.10923307
R6=1.37864607
R7=1.10872404
R8=1.11150394
R9=1.11475423
R10=1.10808438
R11=1.10863249
A3=62.81210991
A4=120.86610698
A5=120.58249588
A6=119.46736692
A7=120.61557606
A8=120.82091235
A9=115.35394955
A10=122.27933972
A11=121.40130502
D4=-101.94501095
D5=106.01032822
D6=106.84534029
D7=-106.00167411
D8=-152.12962712
D9=149.01681348
D10=-31.61490169
D11=179.9388411

1-adamantyl cation **16**

E (B3LYP/6-31G(d)) = -389.8382296 Hartree

E (B3LYP/6-31G(d)) + ZPE = --389.7650237 Hartree

NImag = 0

Final B3LYP/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,2,R3,1,A3
C,3,R4,2,A4,1,D4,0
C,3,R5,2,A5,4,D5,0
C,4,R6,3,A6,2,D6,0
C,6,R7,4,A7,3,D7,0
C,5,R8,3,A8,2,D8,0
H,4,R9,3,A9,6,D9,0
H,4,R10,3,A10,6,D10,0
H,3,R11,2,A11,4,D11,0
H,5,R12,3,A12,8,D12,0
H,5,R13,3,A13,8,D13,0
C,1,R14,2,A14,3,D14,0
H,6,R15,4,A15,7,D15,0
H,7,R16,6,A16,4,D16,0
H,7,R17,6,A17,16,D17,0
C,1,R18,2,A18,14,D18,0
H,8,R19,5,A19,3,D19,0
H,2,R20,1,A20,3,D20,0
H,2,R21,1,A21,3,D21,0
H,14,R22,1,A22,2,D22,0
H,14,R23,1,A23,22,D23,0
H,18,R24,1,A24,2,D24,0
H,18,R25,1,A25,24,D25,0
Variables:
R2=1.4586687
R3=1.62859615
R4=1.53565806
R5=1.53572421
R6=1.53571404
R7=1.53546976
R8=1.5358498
R9=1.09604429
R10=1.09680367
R11=1.09438799
R12=1.0968579
R13=1.09600209
R14=1.4588632
R15=1.09443311
R16=1.09610736
R17=1.09682144
R18=1.45862423
R19=1.09440768
R20=1.09168129
R21=1.09168873
R22=1.09171399
R23=1.09167761
R24=1.09163227
R25=1.09170465
A3=98.93373245
A4=108.14040991
A5=108.12171081
A6=109.83665294
A7=111.48397669
A8=109.82752973
A9=110.81780943
A10=109.44250675
A11=105.31900979
A12=109.43735186
A13=110.79373865
A14=117.7666149

A15=111.75780229
A16=110.7684368
A17=109.47487595
A18=117.78809157
A19=111.74160893
A20=114.2230165
A21=114.24998877
A22=114.20343999
A23=114.20801747
A24=114.24090761
A25=114.21483047
D4=60.395943
D5=-120.76280847
D6=-61.63884914
D7=-57.02220267
D8=61.64956148
D9=122.71425824
D10=-120.16288184
D11=119.62228748
D12=120.18367668
D13=-122.69807294
D14=-75.44203835
D15=-125.8973986
D16=179.61663691
D17=117.10031233
D18=150.89397766
D19=-177.14575234
D20=115.24993668
D21=-115.2939583
D22=-169.29239327
D23=129.44545768
D24=169.24418025
D25=-129.48561024

1-adamantyl cation **16**

E (MP2/6-31G(d)) = -388.4670908 Hartree

E (MP2/6-31G(d)) + ZPE = -388.230484 Hartree

NImag = 0

Final MP2/6-31G(d) structure in terms of initial Z-matrix:

C
C,1,R2
C,1,R3,2,A3
C,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,3,R6,1,A6,2,D6,0
C,4,R7,1,A7,2,D7,0
H,2,R8,1,A8,5,D8,0
H,2,R9,1,A9,5,D9,0
H,3,R10,1,A10,6,D10,0
H,3,R11,1,A11,6,D11,0
H,4,R12,1,A12,7,D12,0
H,4,R13,1,A13,7,D13,0
C,5,R14,2,A14,1,D14,0
C,5,R15,2,A15,14,D15,0
C,6,R16,3,A16,1,D16,0
H,5,R17,2,A17,14,D17,0
H,6,R18,3,A18,16,D18,0
H,7,R19,4,A19,1,D19,0
H,14,R20,5,A20,2,D20,0
H,14,R21,5,A21,20,D21,0
H,15,R22,5,A22,2,D22,0
H,15,R23,5,A23,22,D23,0
H,16,R24,6,A24,3,D24,0
H,16,R25,6,A25,24,D25,0
Variables:
R2=1.45008266
R3=1.45009144
R4=1.44998314
R5=1.61875228
R6=1.61868868
R7=1.61881562
R8=1.09172889
R9=1.09173856
R10=1.09174531
R11=1.09173186
R12=1.09174245
R13=1.09174653
R14=1.52650934
R15=1.52644852
R16=1.52643708
R17=1.0959508
R18=1.09594653
R19=1.09594028
R20=1.09627715
R21=1.09707885
R22=1.0970899
R23=1.09627976
R24=1.09627917
R25=1.09709496
A3=118.0719845
A4=118.05522624
A5=98.26227013
A6=98.2593172
A7=98.26552769
A8=114.3244074
A9=114.3268612
A10=114.32885621
A11=114.32980472
A12=114.3334248
A13=114.33167253
A14=108.23092845
A15=108.21619998
A16=108.23524452

A17=105.11617595
A18=105.12489698
A19=105.10080159
A20=110.81167736
A21=109.40369834
A22=109.39574939
A23=110.81847454
A24=110.81662871
A25=109.39939603
D4=152.65855447
D5=-76.32264506
D6=76.32877928
D7=-76.32866559
D8=114.90685125
D9=-114.89250722
D10=114.91072158
D11=-114.87636749
D12=-114.89603537
D13=114.89303498
D14=60.47881168
D15=-120.98413557
D16=60.49235655
D17=119.51318443
D18=119.50813509
D19=179.99963803
D20=60.88192302
D21=117.33130011
D22=-178.19804599
D23=117.32993635
D24=60.88434469
D25=117.33090779