

Supporting information:

Novel hollow all-carbon structures

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Contents

1	Molecular structures	1	2.16 γ -C ₂₈₈ D_{2h} 2	58
1.1	β -C ₂₈₈	1	2.17 γ -C ₂₈₈ D_{6d} 1	63
1.2	γ -C ₂₈₈	4	2.18 γ -C ₂₈₈ D_{6d} 2	67
2	Molecular coordinates in Å	6	2.19 γ -C ₄₃₂	71
2.1	β -C ₇₂	6	2.20 γ -C ₆₄₈	78
2.2	γ -C ₇₂	7	2.21 β -C ₆₄₈	87
2.3	α -C ₈₀	8	2.22 β -C ₇₂ @C ₂₁₆	97
2.4	β -C ₁₆₂	9	2.23 β -C ₇₂ @C ₂₁₆ @C ₆₄₈	101
2.5	β -C ₂₁₆	12	2.24 β -C ₄ -C ₁₂₀	115
2.6	β -C ₂₈₈ C ₂ 1	15	2.25 β -C ₄ -C ₃₆₀	117
2.7	β -C ₂₈₈ C ₂ 2	19	2.26 γ -C ₄ -C ₁₀₈	122
2.8	β -C ₂₈₈ D_2	24		
2.9	β -C ₂₈₈ D_{3d}	28	1	Molecular structures
2.10	β -C ₂₈₈ D_{3h}	32	1.1	β -C ₂₈₈
2.11	γ -C ₂₈₈ C _{2h}	37		
2.12	γ -C ₂₈₈ C _{2v} 1	41		
2.13	γ -C ₂₈₈ C _{2v} 2	45		
2.14	γ -C ₂₈₈ C _{2v} 3	50		
2.15	γ -C ₂₈₈ D_{2h} 1	54		

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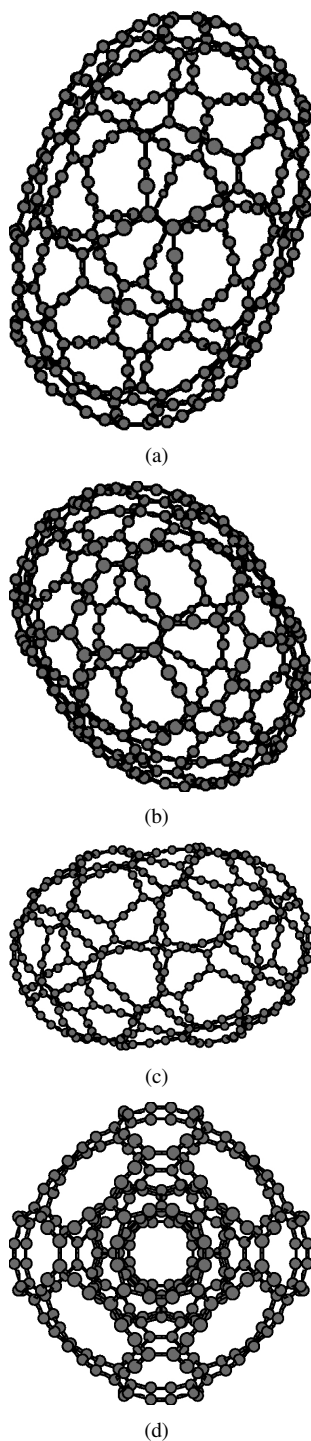


Fig. 1 The molecular structure of β -gaudienes of C_2 and D_2 symmetry β -C₂₈₈ (C_2) #1, β -C₂₈₈ (C_2) #2, β -C₂₈₈ (D_2), and β -C₇₂@ β -C₂₁₆ (O_h).

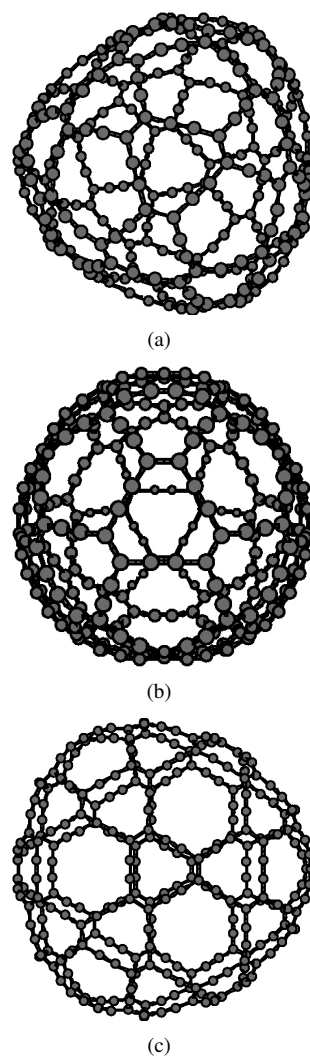


Fig. 2 The molecular structure of β -gaudienes of D_3 , D_{3h} and D_{3d} symmetry β -C₂₈₈ (D_3), β -C₂₈₈ (D_{3h}), and β -C₂₈₈ (D_{3d}).

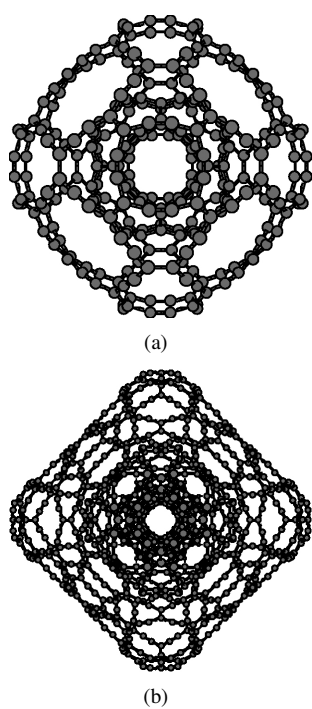
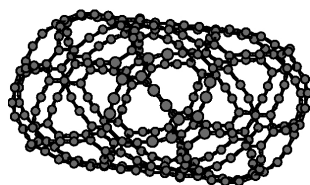
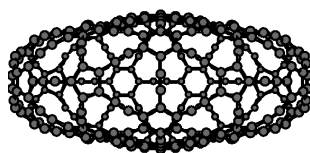


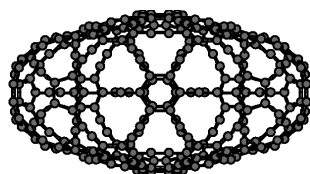
Fig. 3 The molecular structure of β -C₇₂@ β -C₂₁₆ (O_h) and β -C₇₂@ β -C₂₁₆@ β -C₆₄₈ (O_h).

1.2 γ -C₂₈₈

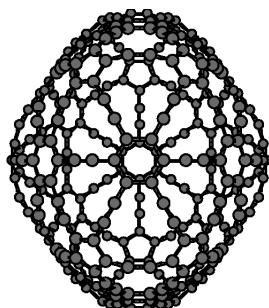
(a)



(b)

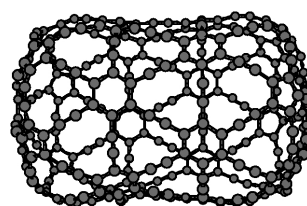


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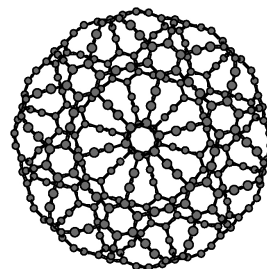


(d)

Fig. 4 The molecular structure of the γ -C₂₈₈ gaudienes (C_{2h}), (C_{2v}) #1, (C_{2v}) #2, and (C_{2v}) #3.



(a)



(b)

Fig. 5 The molecular structure of two γ -C₂₈₈ structures of D_{6d} symmetry. (a) γ -C₂₈₈ (D_{6d}) #1 and (b) (D_{6d}) #2.

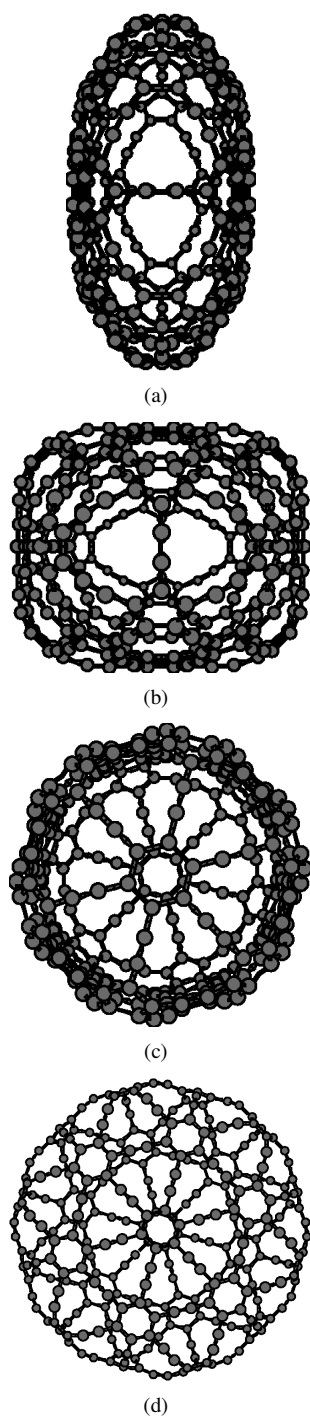


Fig. 6 The molecular structure of the γ -C₂₈₈ gaudienes (D_{2h}) #1, (D_{2h}) #2, (D_{6d}) #1, and (D_{6d}) #2.

2 Molecular coordinates in Å

2.1 β -C₇₂

72

Energy (BP86/SVP) = -2740.248744892 Energy (B3LYP/SVP) = -2738.374865093

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2.2 γ -C₇₂

72

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2.3 α -C₈₀

80

Energy (BP86/SVP) = -3044.728324528 Energy (B3LYP/SVP) = -3042.650148438

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2.4 β -C₁₆₂

162
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C -1.4357079 1.1988834 6.5254184
C -5.9557366 0.6199083 3.3135311
C -5.9557366 -0.6199083 3.3135311
C -0.6258182 4.6047848 5.3751906
C 0.6258182 4.6047848 5.3751906
C -6.5045167 2.0755694 0.8943754
C -6.6264493 1.4471963 -0.1749925

C -1.4357079 -1.1988834 6.5254184
C -2.0480914 -2.2150958 6.1522112
C -4.8940683 -2.5751414 4.2054401
C -3.9384501 -2.9692068 4.9052839
C 2.0480914 2.2150958 6.1522112
C 1.4357079 1.1988834 6.5254184
C 3.9384501 2.9692068 4.9052839
C 4.8940683 2.5751414 4.2054401
C 1.4357079 -1.1988834 6.5254184
C 2.0480914 -2.2150958 6.1522112
C 6.5045167 2.0755694 0.8943754
C 6.6264493 1.4471963 -0.1749925
C 5.9557366 0.6199083 3.3135311
C 5.9557366 -0.6199083 3.3135311
C 5.3150452 1.9815470 -3.3762088
C 5.9684977 1.4123557 -2.4877324
C 1.2232496 3.2674305 -5.7401902
C 2.3054114 2.7029932 -5.4939233
C -1.2232496 3.2674305 -5.7401902
C -2.3054114 2.7029932 -5.4939233
C 3.4816806 0.6212041 -5.1136917
C 3.4816806 -0.6212041 -5.1136917
C -5.3150452 1.9815470 -3.3762088
C -5.9684977 1.4123557 -2.4877324
C -3.4816806 0.6212041 -5.1136917
C -3.4816806 -0.6212041 -5.1136917
C 4.8940683 -2.5751414 4.2054401
C 3.9384501 -2.9692068 4.9052839
C 6.6264493 -1.4471963 -0.1749925
C 6.5045167 -2.0755694 0.8943754
C 5.9684977 -1.4123557 -2.4877324
C 5.3150452 -1.9815470 -3.3762088
C 5.6261914 -4.0784057 1.8686607
C 5.0725008 -5.1603891 1.6153755
C 2.3054114 -2.7029932 -5.4939233
C 1.2232496 -3.2674305 -5.7401902
C 4.3401600 -4.0749372 -3.8854055
C 4.2403708 -5.2203136 -3.4080102
C -2.3054114 -2.7029932 -5.4939233
C -1.2232496 -3.2674305 -5.7401902
C -5.9684977 -1.4123557 -2.4877324
C -5.3150452 -1.9815470 -3.3762088
C -6.6264493 -1.4471963 -0.1749925
C -6.5045167 -2.0755694 0.8943754
C -4.3401600 -4.0749372 -3.8854055
C -4.2403708 -5.2203136 -3.4080102
C -5.6261914 -4.0784057 1.8686607
C -5.0725008 -5.1603891 1.6153755
C 0.6258182 -4.6047848 5.3751906
C -0.6258182 -4.6047848 5.3751906
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C 2.9540460 -6.1109228 3.2803259
C -2.5625806 -5.4105655 4.2264314
C -2.9540460 -6.1109228 3.2803259
C 4.3363469 -6.5561396 -0.1715534
C 4.2499761 -6.5844625 -1.4126311
C 2.2273632 -7.6030133 1.5620327
C 1.2051780 -8.1493342 1.1049619
C 1.1728816 -6.0600886 -5.0702750
C 2.0233979 -6.6590294 -4.3876970
C -1.1728816 -6.0600886 -5.0702750
C -2.0233979 -6.6590294 -4.3876970
C 2.0420148 -8.0704122 -2.4822482
C 1.1762751 -8.5594449 -1.7316659
C -4.2499761 -6.5844625 -1.4126311
C -4.3363469 -6.5561396 -0.1715534
C -2.0420148 -8.0704122 -2.4822482
C -1.1762751 -8.5594449 -1.7316659

C -1.2051780 -8.1493342 1.1049619
 C -2.2273632 -7.6030133 1.5620327

2.5 β -C₂₁₆

216

Energy (BP86/SVP) = -8221.218661131 Energy (B3LYP/SVP) = -8215.586263054

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 C 1.9442221 1.9442221 -8.4305603
 C -1.9442221 1.9442221 -8.4305603
 C 0.7370811 -5.7222849 -5.7222849
 C -0.7370811 -5.7222849 -5.7222849
 C 2.7546017 -2.7546017 -7.5249100
 C -2.7546017 -2.7546017 -7.5249100
 C 1.9442221 -8.4305603 -1.9442221
 C -1.9442221 -8.4305603 -1.9442221
 C 2.7546017 -7.5249100 -2.7546017
 C -2.7546017 -7.5249100 -2.7546017
 C 1.9442221 -8.4305603 1.9442221
 C -1.9442221 -8.4305603 1.9442221
 C 5.7222849 -0.7370811 -5.7222849
 C 5.7222849 0.7370811 -5.7222849
 C 2.7546017 2.7546017 -7.5249100
 C 5.7222849 -5.7222849 -0.7370811
 C 7.5249100 -2.7546017 -2.7546017
 C 2.7546017 -7.5249100 2.7546017
 C 5.7222849 -5.7222849 0.7370811
 C 0.7370811 -5.7222849 5.7222849
 C -0.7370811 -5.7222849 5.7222849
 C -2.7546017 -7.5249100 2.7546017
 C 8.4305603 -1.9442221 -1.9442221
 C 8.4305603 1.9442221 -1.9442221
 C 7.5249100 2.7546017 -2.7546017
 C 7.5249100 -2.7546017 2.7546017
 C 8.4305603 -1.9442221 1.9442221
 C 2.7546017 -2.7546017 7.5249100
 C 5.7222849 -0.7370811 5.7222849
 C 1.9442221 -1.9442221 8.4305603
 C -1.9442221 -1.9442221 8.4305603
 C -2.7546017 -2.7546017 7.5249100
 C 8.4305603 1.9442221 1.9442221
 C 5.7222849 0.7370811 5.7222849
 C 7.5249100 2.7546017 2.7546017
 C 1.9442221 1.9442221 8.4305603
 C 2.7546017 2.7546017 7.5249100
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 C 5.7222849 5.7222849 0.7370811
 C 5.7222849 5.7222849 -0.7370811
 C 0.7370811 5.7222849 5.7222849
 C 2.7546017 7.5249100 2.7546017
 C -2.7546017 2.7546017 7.5249100
 C -0.7370811 5.7222849 5.7222849
 C -5.7222849 -0.7370811 5.7222849
 C -5.7222849 0.7370811 5.7222849
 C -5.7222849 -5.7222849 0.7370811
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 C -5.7222849 -5.7222849 -0.7370811
 C 2.7546017 7.5249100 -2.7546017
 C 0.7370811 5.7222849 -5.7222849
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 C 1.9442221 8.4305603 -1.9442221
 C -2.7546017 7.5249100 2.7546017
 C -1.9442221 8.4305603 1.9442221
 C -7.5249100 2.7546017 2.7546017
 C -5.7222849 5.7222849 0.7370811
 C -8.4305603 -1.9442221 1.9442221

C -8.4305603 1.9442221 1.9442221
C -7.5249100 -2.7546017 -2.7546017
C -8.4305603 -1.9442221 -1.9442221
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C -0.7370811 5.7222849 -5.7222849
C -2.7546017 2.7546017 -7.5249100
C -1.9442221 8.4305603 -1.9442221
C -2.7546017 7.5249100 -2.7546017
C -5.7222849 5.7222849 -0.7370811
C -8.4305603 1.9442221 -1.9442221
C -7.5249100 2.7546017 -2.7546017
C -5.7222849 0.7370811 -5.7222849
C 0.6220624 -2.2864649 -8.7274399
C -0.6220624 -2.2864649 -8.7274399
C 2.2864649 -0.6220624 -8.7274399
C 2.2864649 0.6220624 -8.7274399
C -2.2864649 -0.6220624 -8.7274399
C -2.2864649 0.6220624 -8.7274399
C 0.6220624 2.2864649 -8.7274399
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C 2.1803651 -3.9217792 -7.0065537
C 1.4709506 -6.4793869 -4.7994800
C 2.1803651 -7.0065537 -3.9217792
C -1.4709506 -4.7994800 -6.4793869
C -2.1803651 -3.9217792 -7.0065537
C -1.4709506 -6.4793869 -4.7994800
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C -0.6220624 -8.7274399 -2.2864649
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C 2.1803651 3.9217792 -7.0065537
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C 6.4793869 -4.7994800 -1.4709506
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C 8.7274399 -2.2864649 0.6220624
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C 8.7274399 2.2864649 0.6220624
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C 7.0065537 -2.1803651 3.9217792
C 6.4793869 -1.4709506 4.7994800
C 8.7274399 -0.6220624 2.2864649
C 8.7274399 0.6220624 2.2864649
C 3.9217792 -2.1803651 7.0065537
C 4.7994800 -1.4709506 6.4793869
C 0.6220624 -2.2864649 8.7274399
C -0.6220624 -2.2864649 8.7274399
C 2.2864649 -0.6220624 8.7274399
C 2.2864649 0.6220624 8.7274399
C -2.2864649 -0.6220624 8.7274399
C -2.2864649 0.6220624 8.7274399
C -3.9217792 -2.1803651 7.0065537
C -4.7994800 -1.4709506 6.4793869
C 6.4793869 1.4709506 4.7994800
C 7.0065537 2.1803651 3.9217792
C 4.7994800 1.4709506 6.4793869
C 3.9217792 2.1803651 7.0065537
C 7.0065537 3.9217792 2.1803651
C 6.4793869 4.7994800 1.4709506
C 0.6220624 2.2864649 8.7274399
C -0.6220624 2.2864649 8.7274399
C 2.1803651 3.9217792 7.0065537
C 1.4709506 4.7994800 6.4793869
C 4.7994800 6.4793869 1.4709506
C 3.9217792 7.0065537 2.1803651
C 4.7994800 6.4793869 -1.4709506
C 3.9217792 7.0065537 -2.1803651
C 1.4709506 6.4793869 4.7994800
C 2.1803651 7.0065537 3.9217792
C -2.1803651 3.9217792 7.0065537
C -1.4709506 4.7994800 6.4793869
C -3.9217792 2.1803651 7.0065537
C -4.7994800 1.4709506 6.4793869
C -1.4709506 6.4793869 4.7994800
C -2.1803651 7.0065537 3.9217792
C -6.4793869 -1.4709506 4.7994800
C -7.0065537 -2.1803651 3.9217792
C -6.4793869 1.4709506 4.7994800
C -7.0065537 2.1803651 3.9217792
C -6.4793869 -4.7994800 1.4709506
C -7.0065537 -3.9217792 2.1803651
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C -7.0065537 -3.9217792 -2.1803651
C 2.1803651 7.0065537 -3.9217792
C 1.4709506 6.4793869 -4.7994800
C 2.2864649 8.7274399 0.6220624
C 2.2864649 8.7274399 -0.6220624
C 0.6220624 8.7274399 2.2864649
C -0.6220624 8.7274399 2.2864649
C 0.6220624 8.7274399 -2.2864649
C -0.6220624 8.7274399 -2.2864649
C -3.9217792 7.0065537 2.1803651
C -4.7994800 6.4793869 1.4709506
C -2.2864649 8.7274399 0.6220624
C -2.2864649 8.7274399 -0.6220624
C -7.0065537 3.9217792 2.1803651
C -6.4793869 4.7994800 1.4709506
C -8.7274399 -0.6220624 2.2864649
C -8.7274399 0.6220624 2.2864649

C -8.7274399 -2.2864649 0.6220624
 C -8.7274399 -2.2864649 -0.6220624
 C -8.7274399 2.2864649 0.6220624
 C -8.7274399 2.2864649 -0.6220624
 C -7.0065537 -2.1803651 -3.9217792
 C -6.4793869 -1.4709506 -4.7994800
 C -8.7274399 -0.6220624 -2.2864649
 C -8.7274399 0.6220624 -2.2864649
 C -1.4709506 4.7994800 -6.4793869
 C -2.1803651 3.9217792 -7.0065537
 C -1.4709506 6.4793869 -4.7994800
 C -2.1803651 7.0065537 -3.9217792
 C -3.9217792 2.1803651 -7.0065537
 C -4.7994800 1.4709506 -6.4793869
 C -3.9217792 7.0065537 -2.1803651
 C -4.7994800 6.4793869 -1.4709506
 C -6.4793869 4.7994800 -1.4709506
 C -7.0065537 3.9217792 -2.1803651
 C -7.0065537 2.1803651 -3.9217792
 C -6.4793869 1.4709506 -4.7994800

2.6 β -C₂₈₈ C₂ 1

288
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 C 5.9731107 8.6522492 -2.2878190
 C 2.8373314 11.0834416 -1.8232281
 C 7.4241906 8.0992574 1.3872322
 C 5.0409187 9.8057087 4.0868640
 C 2.1130243 11.5757951 2.0578896
 C 3.1509823 7.6645514 -6.1448448
 C 2.0350749 8.5742930 -5.9432650
 C 6.0373320 7.6349819 -3.3404171
 C 1.7311691 10.9803337 -2.7731624
 C 1.1600667 4.1595454 -8.8802503
 C -1.9365780 6.3273571 -7.6296276
 C 2.5050252 4.3453615 -8.3416111
 C -1.7119309 7.5265111 -6.8483113
 C -0.4218183 0.5959865 -9.7295528
 C -4.9084102 3.8460579 -6.6412504
 C -4.0861564 0.2611011 -8.2181783
 C 7.7785978 4.1237875 -2.4665893
 C 8.0648270 6.8224331 1.6986331
 C 8.2969721 3.9731867 -1.0977160
 C 4.6171492 0.9949895 -7.6915742
 C 6.9770326 0.6949958 -4.4394714
 C 4.0861564 -0.2611011 -8.2181783
 C 0.4218183 -0.5959865 -9.7295528
 C 7.4733704 5.0674435 5.2164412
 C 4.7568334 9.1071660 5.3379697
 C 6.5378125 5.6478832 6.1746732
 C 8.3260206 0.4511046 0.7939147
 C 7.5645629 1.1082627 4.6589849
 C 7.1515415 -0.6052737 -3.7919940
 C 7.9961675 -0.8186435 0.1321828
 C 4.9084102 -3.8460579 -6.6412504
 C 5.6743250 -4.0032875 -5.4061527
 C 1.9365780 -6.3273571 -7.6296276
 C -1.1600667 -4.1595454 -8.8802503
 C 0.9920019 8.7478759 6.5745347
 C 0.7239203 11.4916820 2.5457981
 C -0.0829051 9.3615341 5.8061556
 C 3.9706420 3.1926946 8.0053758
 C 0.4702266 5.0946270 8.1145060
 C 6.7706315 0.1556975 5.4322097
 C 4.0363076 1.7392613 7.8891743
 C 6.6984509 -3.8130958 2.4915793

C 6.2743873 -3.5208394 3.8609396
C 5.0584889 -7.3438836 -3.2471122
C 5.5463122 -7.2637857 0.7353946
C 4.0973090 -8.3286263 -3.7626560
C 1.7119309 -7.5265111 -6.8483113
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C -2.0140086 10.8315628 -1.4513783
C -3.4530578 7.2920703 5.1845418
C -4.8146597 8.2277869 1.5492480
C -0.7883299 4.3513323 7.9890802
C -3.6949930 5.9748486 5.7666435
C 0.6443007 -0.3490143 8.4838464
C -0.6443007 0.3490143 8.4838464
C 3.6949930 -5.9748486 5.7666435
C 0.7883299 -4.3513323 7.9890802
C 4.8146597 -8.2277869 1.5492480
C 3.4530578 -7.2920703 5.1845418
C 2.0140086 -10.8315628 -1.4513783
C 2.2562388 -10.8781787 -0.0102697
C -2.0350749 -8.5742930 -5.9432650
C -1.7311691 -10.9803337 -2.7731624
C -4.0973090 8.3286263 -3.7626560
C -5.5463122 7.2637857 0.7353946
C -5.0584889 7.3438836 -3.2471122
C -6.2743873 3.5208394 3.8609396
C -6.6984509 3.8130958 2.4915793
C -4.0363076 -1.7392613 7.8891743
C -6.7706315 -0.1556975 5.4322097
C -0.4702266 -5.0946270 8.1145060
C -3.9706420 -3.1926946 8.0053758
C 0.0829051 -9.3615341 5.8061556
C -0.9920019 -8.7478759 6.5745347
C -0.7239203 -11.4916820 2.5457981
C -5.6743250 4.0032875 -5.4061527
C -7.9961675 0.8186435 0.1321828
C -7.1515415 0.6052737 -3.7919940
C -7.5645629 -1.1082627 4.6589849
C -8.3260206 -0.4511046 0.7939147
C -6.5378125 -5.6478832 6.1746732
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C -4.7568334 -9.1071660 5.3379697
C -6.9770326 -0.6949958 -4.4394714
C -4.6171492 -0.9949895 -7.6915742
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C -7.7785978 -4.1237875 -2.4665893
C -8.0648270 -6.8224331 1.6986331
C -2.5050252 -4.3453615 -8.3416111
C -6.0373320 -7.6349819 -3.3404171
C -3.1509823 -7.6645514 -6.1448448
C -5.9731107 -8.6522492 -2.2878190
C -7.4241906 -8.0992574 1.3872322
C -2.8373314 -11.0834416 -1.8232281
C -5.0409187 -9.8057087 4.0868640
C -2.1130243 -11.5757951 2.0578896
C 5.0036825 9.6689518 -2.3062871
C 4.0528533 10.4481145 -2.1249573
C 6.6906093 8.5290355 -1.0988349
C 7.1332663 8.4060370 0.0590015
C 2.6117375 11.5245068 -0.5198395
C 2.3730233 11.6901610 0.6917478
C 6.8326764 8.8629364 2.4056005
C 6.0944713 9.3843253 3.2579826
C 4.0878346 10.6527386 3.5212491
C 3.1720058 11.2115597 2.8882773
C 4.2735425 7.7392028 -5.3042341
C 5.1610273 7.7217448 -4.4344513
C 3.0120791 6.5702543 -7.0120205
C 2.8220779 5.5453476 -7.6878781

C 2.0648515 9.5646259 -4.9604569
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288
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C -7.0757219 -2.4878200 -3.6153348
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C -8.1275924 0.8043745 -3.0766624
C -7.9384363 -0.3978153 -2.8130852
C -4.0590870 -7.3696259 -1.2205577
C -3.0825347 -8.1305269 -1.1054189
C -6.9812019 -3.4843934 -0.8779874
C -6.3599874 -4.5084274 -0.5387851
C -8.0227886 -1.4718779 -0.1091980
C -8.3330939 -0.7976843 0.8888201
C -5.0638025 -5.9071512 1.0072871
C -4.5080100 -6.1680538 2.0888017
C -8.3000952 -0.3128075 3.2718661
C -7.9431707 -0.5968264 4.4314406
C 0.2764186 -9.3085709 0.0674723
C 1.4978707 -9.4933194 -0.0788517
C -1.6017775 -8.3809520 1.3182122
C -2.1133316 -7.8129689 2.3039621
C 3.7437524 -9.1708102 0.7732881
C 4.4931369 -8.7697190 1.6825131
C -4.3153570 -5.6143734 4.4171259
C -4.7248709 -4.8975346 5.3506100
C -1.8358799 -7.1094994 4.5830208
C -1.0784216 -7.0252298 5.5646083
C -6.7470858 -2.0419917 5.9751782
C -6.0146582 -3.0220122 6.1927997
C -6.6014999 0.1383100 7.8598809
C -5.8451629 0.1859064 8.8449319
C 4.7892840 -7.9057004 3.9293670
C 4.3112417 -7.5604594 5.0224496
C 1.1453593 -7.0560154 6.5654079
C 2.3787507 -7.1515968 6.4381104
C -3.1386123 -4.8960721 7.7119820
C -2.0524780 -5.4970444 7.7585457
C -4.3847851 -3.0663393 8.6005381
C -4.3069088 -2.1244120 9.4111993
C 0.1113973 -5.4688083 8.7633118
C 0.8134225 -4.8181400 9.5545733
C -2.8734916 -0.8482652 10.8600782
C -1.7202094 -0.7348972 11.3088907
C 0.9892955 -2.8362780 10.9081322
C 0.3975319 -1.8223385 11.3206424

2.8 β -C₂₈₈ D₂

288

Energy (BP86/SVP) = -10961.91928794 Energy (B3LYP/SVP) = -10954.43766883

C -4.4089263 -0.6267253 7.7257508
 C -7.2762232 1.8320848 6.3484127
 C -8.0409561 -3.5879229 6.1194931
 C -9.1179879 -2.6980396 5.6875142
 C -4.6695737 -2.0667793 7.6284491
 C -8.5436913 1.2428285 5.9004925
 C -0.5446623 0.4912255 7.9886931
 C 0.3011674 4.2806439 6.9582938
 C -6.1359744 5.2842878 4.6402214
 C -2.2597289 6.3936098 4.6767877
 C -7.0463112 -6.7618731 3.9525570
 C -10.7385337 -4.6527301 1.5523616
 C -11.1726387 -3.5441092 2.3879757
 C -7.7117580 -6.9878421 2.6677429
 C -1.7081024 -4.6569184 6.9032374
 C -3.1101408 -7.3397914 4.3035402
 C 0.5446623 -0.4912255 7.9886931
 C -0.3011674 -4.2806439 6.9582938
 C 4.6695737 2.0667793 7.6284491
 C 1.7081024 4.6569184 6.9032374
 C 4.4089263 0.6267253 7.7257508
 C 8.0409561 3.5879229 6.1194931
 C 3.1101408 7.3397914 4.3035402
 C 7.0463112 6.7618731 3.9525570
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 C -12.2621705 0.0793688 -0.7220826
 C -12.2621705 -0.0793688 0.7220826
 C -10.7804461 -2.8322034 -2.9959719
 C -5.4197613 -7.8255616 -0.4835845
 C -6.9889761 -5.8514374 -3.5860579
 C -2.2554121 -7.8174821 3.2134045
 C -3.9843855 -8.0799680 -0.3848523
 C 2.2597289 -6.3936098 4.6767877
 C 1.7156389 -7.2297140 3.6008350
 C 7.2762232 -1.8320848 6.3484127
 C 6.1359744 -5.2842878 4.6402214
 C 8.5436913 -1.2428285 5.9004925
 C 9.1179879 2.6980396 5.6875142
 C -11.1726387 3.5441092 -2.3879757
 C -10.7385337 4.6527301 -1.5523616
 C -10.3580057 4.0844696 2.3777673
 C -10.7804461 2.8322034 2.9959719
 C -8.5436913 -1.2428285 -5.9004925
 C -9.1179879 2.6980396 -5.6875142
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 C -2.2597289 -6.3936098 -4.6767877
 C 3.9843855 -8.0799680 0.3848523
 C 2.2554121 -7.8174821 -3.2134045
 C 6.9889761 -5.8514374 3.5860579
 C 5.4197613 -7.8255616 0.4835845
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 C 10.3580057 -4.0844696 2.3777673
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 C -7.0463112 6.7618731 -3.9525570
 C -4.4089263 0.6267253 -7.7257508
 C -4.6695737 2.0667793 -7.6284491
 C 0.3011674 -4.2806439 -6.9582938

C -0.5446623 -0.4912255 -7.9886931
C 3.1101408 -7.3397914 -4.3035402
C 1.7081024 -4.6569184 -6.9032374
C 7.7117580 -6.9878421 -2.6677429
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C -1.7081024 4.6569184 -6.9032374
C -3.1101408 7.3397914 -4.3035402
C 0.5446623 0.4912255 -7.9886931
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C -2.2554121 7.8174821 -3.2134045
C -3.9843855 8.0799680 0.3848523
C 2.2597289 6.3936098 -4.6767877
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C 3.9843855 8.0799680 -0.3848523
C 2.2554121 7.8174821 3.2134045
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C -5.9314742 -2.5691412 7.3126368
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C -7.5795710 -5.8548508 4.8753864
C -9.0457543 -1.3376797 5.9989581
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C -2.5544271 -6.6172527 5.3673132

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C 5.9314742 2.5691412 7.3126368
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C 2.1243994 5.7784163 6.1759862
C 2.5544271 6.6172527 5.3673132
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C 7.5795710 5.8548508 4.8753864
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C -6.4555581 -6.7438974 -2.6483112
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C 0.3459680 -7.4943482 3.5122110
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C 4.8137598 -5.7251424 4.7421473
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C 3.1955207 -7.9350606 1.5323470
C 6.9313726 -3.1201452 5.9212020
C 6.5796309 -4.1922749 5.3934253
C 8.8190287 0.1162001 6.0759358
C 9.0457543 1.3376797 5.9989581
C 9.4242646 -1.9378578 5.0651603
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C -8.2659721 5.3522329 3.3383772
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C -6.9313726 -3.1201452 -5.9212020
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C 6.4555581 -6.7438974 2.6483112
C 5.9729203 -7.3617047 1.6837683
C 8.2659721 -5.3522329 3.3383772
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C 12.0393243 -1.0235582 1.5602704
C 10.7554558 -4.4057617 1.0683297
C 10.8800445 -4.5771381 -0.1541906
C 12.1387081 1.3518973 1.2989492
C 11.8051089 2.4291574 1.8174539
C -6.9838577 7.5483362 -1.6130997
C -6.2418326 7.7968545 -0.6465300
C -5.9729203 7.3617047 1.6837683
C -6.4555581 6.7438974 2.6483112
C -7.8886244 4.8571744 -5.5502873
C -7.5795710 5.8548508 -4.8753864
C -6.9730947 3.0732610 -6.8563540
C -5.9314742 2.5691412 -7.3126368
C -5.7294126 7.1803075 -4.1347327
C -4.4997955 7.3551643 -4.2112859
C -3.0908762 0.2016355 -7.9128972
C -1.8851900 -0.0962952 -7.9856329
C -3.6105131 2.9809923 -7.6116369
C -2.6978139 3.7928112 -7.3823701
C -0.0510883 -3.0356012 -7.4919302
C -0.2663778 -1.8528213 -7.8101383
C 2.5544271 -6.6172527 -5.3673132
C 2.1243994 -5.7784163 -6.1759862
C 4.4997955 -7.3551643 -4.2112859
C 5.7294126 -7.1803075 -4.1347327
C 2.6978139 -3.7928112 -7.3823701
C 3.6105131 -2.9809923 -7.6116369
C 8.9278695 -6.3663374 -2.3832603
C 9.8733081 -5.6307322 -2.0462229
C 7.5795710 -5.8548508 -4.8753864
C 7.8886244 -4.8571744 -5.5502873
C -2.1243994 5.7784163 -6.1759862
C -2.5544271 6.6172527 -5.3673132
C 0.2663778 1.8528213 -7.8101383
C 0.0510883 3.0356012 -7.4919302
C 1.8851900 0.0962952 -7.9856329
C 3.0908762 -0.2016355 -7.9128972
C 0.6433318 5.0859100 -6.3066477
C 1.4002059 5.7565536 -5.5836222
C 5.9314742 -2.5691412 -7.3126368
C 6.9730947 -3.0732610 -6.8563540
C 5.4324367 0.2806092 -7.4268934
C 6.3242406 1.0357488 -6.9974819
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C -3.3768839 8.2410647 -0.8674021
C -0.8692949 7.7064168 -3.3512968
C 0.3459680 7.4943482 -3.5122110
C -3.1955207 7.9350606 1.5323470
C -2.5309575 7.6508985 2.5438092
C 3.6204749 6.0795515 -4.7205144
C 4.8137598 5.7251424 -4.7421473
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C 3.1955207 7.9350606 -1.5323470
C 6.9313726 3.1201452 -5.9212020
C 6.5796309 4.1922749 -5.3934253
C 9.0457543 -1.3376797 -5.9989581
C 8.8190287 -0.1162001 -6.0759358
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C 10.6739222 -3.3974354 -3.6881300

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C 12.1387081 -1.3518973 -1.2989492
C -0.3459680 7.4943482 3.5122110
C 0.8692949 7.7064168 3.3512968
C 3.3768839 8.2410647 0.8674021
C 2.8318142 8.1630783 1.9841229
C 6.4555581 6.7438974 -2.6483112
C 5.9729203 7.3617047 -1.6837683
C 8.2659721 5.3522329 -3.3383772
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C 6.9838577 7.5483362 1.6130997
C 11.5727670 1.9228190 -2.2810857
C 12.0393243 1.0235582 -1.5602704
C 10.7554558 4.4057617 -1.0683297
C 10.8800445 4.5771381 0.1541906
C 8.9278695 6.3663374 2.3832603
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2.9 β -C₂₈₈ D_{3d}

288

Energy (BP86/SVP) = -10961.93905124 Energy (B3LYP/SVP) = -10954.45260731

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C 5.8855479 0.2469716 -9.5575099
C 7.7517835 0.7612315 -5.0581212
C 5.8492215 -3.3770496 -7.8935937
C 8.0248713 -0.6190664 -0.3915088
C 7.0078026 -4.0459567 1.4484700
C 4.3811340 -6.4730958 -4.4183728
C 4.5485629 -6.6402092 -0.3915088
C 4.3666286 4.8167239 -8.7476635
C 1.9982882 1.9912618 -11.9321246
C 2.7236274 0.7349374 -11.9321246
C 3.1566576 4.9735482 -9.5575099
C 7.0050230 4.0443519 -2.9031274
C 4.5351375 6.3326257 -5.0581212
C 8.0248713 0.6190664 0.3915088
C 7.0078026 4.0459567 -1.4484700
C 7.7517835 -0.7612315 5.0581212
C 7.0050230 -4.0443519 2.9031274
C 7.7964325 0.5576254 4.4183728
C 6.3547196 -1.3732493 8.7476635
C 4.3666286 -4.8167239 8.7476635
C 4.5351375 -6.3326257 5.0581212
C -1.9982882 1.9912618 -11.9321246
C -2.7236274 0.7349374 -11.9321246
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C 0.7253392 -2.7261992 -11.9321246
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C -3.1566576 4.9735482 -9.5575099
C 3.4152984 7.0307213 -4.4183728
C 0.0000000 7.2562444 -6.5157828
C 4.5485629 6.6402092 0.3915088
C 3.4763084 7.2592756 -0.3915088
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C 4.3811340 6.4730958 4.4183728
C 5.8492215 3.3770496 7.8935937
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C -5.8855479 0.2469716 -9.5575099
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C -2.7288903 -5.2205198 -9.5575099
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C -6.3547196 1.3732493 -8.7476635
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C -0.0000000 8.0887038 2.9031274
C 2.7288903 5.2205198 9.5575099
C 1.9880910 6.1899733 8.7476635
C 0.7253392 2.7261992 11.9321246
C 2.7236274 -0.7349374 11.9321246
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C -7.0078026 4.0459567 -1.4484700
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C -4.3811340 6.4730958 4.4183728
C -1.9880910 6.1899733 8.7476635
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C -2.7288903 5.2205198 9.5575099
C -5.8492215 3.3770496 7.8935937
C -0.7253392 2.7261992 11.9321246
C 2.7288903 -5.2205198 -9.5575099
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 C -1.2086996 -7.3802242 5.8188291
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 C 3.4427345 -7.2074812 3.0316742
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 C 2.2639390 -7.3164018 5.1609615

2.10 β -C₂₈₈ D_{3h}

288

Energy (BP86/SVP) = -10961.88323319 Energy (B3LYP/SVP) = -10954.38680284

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 C -8.7610000 -2.0064457 4.1893791
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 C -8.8470912 6.4217728 -1.9729584
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C 4.9616498 7.3500627 4.3146894
C 1.2106837 10.2163211 2.9417251
C 0.1156983 10.6352055 2.5276492
C 3.4382869 9.9144157 2.2272595
C 4.1427978 10.0099066 1.2069431
C -1.2072858 11.2462175 0.6220265
C -1.2072858 11.2462175 -0.6220265
C 10.9082560 2.1554595 2.0771719
C 11.3563745 1.1855818 1.4422372
C 8.2422517 6.1566434 2.9417251
C 9.1525090 5.4178004 2.5276492
C 6.8669924 7.9348516 2.2272595
C 6.5974345 8.5927214 1.2069431
C 10.3431530 4.5775686 0.6220265
C 10.3431530 4.5775686 -0.6220265
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C 6.5974345 8.5927214 -1.2069431
C 6.8669924 7.9348516 -2.2272595
C 0.1156983 10.6352055 -2.5276492
C 1.2106837 10.2163211 -2.9417251
C -4.6514433 10.4276998 -1.4422372
C -3.5874453 10.5245566 -2.0771719
C -6.7049313 9.2421179 -1.4422372
C -7.3208107 8.3690971 -2.0771719
C -2.1878507 9.5570341 -3.7816328
C -2.0207732 8.5979229 -4.5577003

C -7.1827089 6.6732514 -3.7816328
C -6.4356330 6.0490024 -4.5577003
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C 9.1525090 5.4178004 -2.5276492
C 3.8845162 7.9719461 -4.3146894
C 4.9616498 7.3500627 -4.3146894
C 1.5275804 8.0247638 -4.8221120
C 0.5262753 7.4099215 -5.2307947
C 6.1858591 5.3353053 -4.8221120
C 6.1540426 4.1607285 -5.2307947
C -3.1403151 6.6814942 -5.4133703
C -4.2161862 6.0603397 -5.4133703
C -0.6522862 5.3805366 -5.9219511
C -0.7129640 4.1544087 -6.1398667
C 10.9082560 2.1554595 -2.0771719
C 11.3563745 1.1855818 -1.4422372
C 9.3705597 2.8837827 -3.7816328
C 8.4564062 2.5489205 -4.5577003
C 11.3563745 -1.1855818 -1.4422372
C 10.9082560 -2.1554595 -2.0771719
C 4.9858245 2.1253719 -5.9219511
C 3.9543055 1.4597594 -6.1398667
C 7.3565013 0.6211545 -5.4133703
C 7.3565013 -0.6211545 -5.4133703
C 0.4685899 2.0551776 -6.3578158
C 1.5455411 1.4333996 -6.3578158
C -4.3335383 3.2551647 -5.9219511
C -3.2413414 2.6946493 -6.1398667
C -6.6803179 3.2491930 -5.2307947
C -7.7134395 2.6894585 -4.8221120
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C -2.0141310 -0.6217780 -6.3578158
C -8.8461660 0.6218834 -4.3146894
C -8.8461660 -0.6218834 -4.3146894
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C 8.4564062 -2.5489205 -4.5577003
C 3.9543055 -1.4597594 -6.1398667
C 4.9858245 -2.1253719 -5.9219511
C 1.5455411 -1.4333996 -6.3578158
C 0.4685899 -2.0551776 -6.3578158
C 6.1540426 -4.1607285 -5.2307947
C 6.1858591 -5.3353053 -4.8221120
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C -4.3335383 -3.2551647 -5.9219511
C -0.7129640 -4.1544087 -6.1398667
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C -7.7134395 -2.6894585 -4.8221120
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C -9.2682073 -5.2174051 -2.5276492
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C 1.5275804 -8.0247638 -4.8221120
C -4.2161862 -6.0603397 -5.4133703
C -3.1403151 -6.6814942 -5.4133703
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C -7.1827089 -6.6732514 -3.7816328
C -2.0207732 -8.5979229 -4.5577003
C -2.1878507 -9.5570341 -3.7816328
C -7.3208107 -8.3690971 -2.0771719
C -6.7049313 -9.2421179 -1.4422372
C -3.5874453 -10.5245566 -2.0771719
C -4.6514433 -10.4276998 -1.4422372

2.11 γ -C₂₈₈ C_{2h}

288

Energy (BP86/SVP) = -10963.86993818 Energy (B3LYP/SVP) = -10956.35458406

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C 6.2017303 -2.4611424 5.8920249
C 8.1815589 -1.2935023 4.9577861
C 8.5131277 -2.4948273 4.2095530
C 6.3977351 -3.5730967 4.9999529
C 7.5972037 -3.6188498 4.2087885
C 3.7559465 2.1152349 7.3997395
C 2.6187872 -1.2526073 9.0958429
C 4.9351115 2.0761805 6.5865430
C 3.0769758 -2.4209488 8.3955086
C -0.8202728 2.7480785 8.8873408
C -1.2454698 1.4820687 9.4758195
C 2.7375045 3.1130642 7.1336861
C 1.2454698 -1.4820687 9.4758195
C -1.9550142 3.3233167 8.2356739
C -3.0769758 2.4209488 8.3955086
C -2.6187872 1.2526073 9.0958429
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C 11.0776953 -2.0805121 1.1781648
C 11.5686395 -0.7970979 -0.7280446
C 11.0776953 -2.0805121 -1.1781648
C 10.8802285 -2.9046759 0.0000000
C 9.6380230 2.2122928 3.7549755
C 10.5425040 2.4201579 2.6575887
C 5.1325412 3.1165060 5.6119127
C 8.6616827 3.2728078 3.7191989
C 2.8239532 3.9433694 5.9510465
C 4.0441891 3.9671427 5.2030477
C -0.4827984 5.4274403 4.1390934
C -1.7752831 5.2873940 4.7745905
C 8.9022544 4.0980706 2.5642178
C 10.0987550 3.6053345 1.9282844
C 4.3465699 5.4193774 1.4401108
C 5.5929365 5.3853866 0.7256610
C -0.4023501 5.7839561 2.7512298
C 3.1137197 5.6188698 0.7184292
C -1.6097410 6.0810591 2.0209381
C -2.8819534 6.0201177 2.6916968
C -2.9842524 5.4999150 4.0307085
C 10.0987550 3.6053345 -1.9282844
C 10.5425040 2.4201579 -2.6575887
C 5.5929365 5.3853866 -0.7256610
C 8.9022544 4.0980706 -2.5642178
C 3.1137197 5.6188698 -0.7184292
C 4.3465699 5.4193774 -1.4401108
C -1.6097410 6.0810591 -2.0209381
C -0.4023501 5.7839561 -2.7512298
C -6.3162116 6.6375668 -0.7255446
C -6.3162116 6.6375668 0.7255446
C -2.8819534 6.0201177 -2.6916968
C -7.5922679 6.1787290 -1.1757126
C -8.4010940 5.9294365 0.0000000
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C 8.6616827 3.2728078 -3.7191989
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C 4.0441891 3.9671427 -5.2030477
C 5.1325412 3.1165060 -5.6119127
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C -6.3977351 3.5730967 -4.9999529
C -11.0776953 2.0805121 -1.1781648

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C -11.5686395 0.7970979 0.7280446
C -11.0776953 2.0805121 1.1781648
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C 7.0097681 -1.2659939 -5.7751504
C 2.7375045 3.1130642 -7.1336861
C 3.7559465 2.1152349 -7.3997395
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C 1.2454698 -1.4820687 -9.4758195
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C -5.5929365 -5.3853866 0.7256610
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C -8.1815589 1.2935023 4.9577861
C -7.5972037 3.6188498 4.2087885
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C 0.4827984 -5.4274403 4.1390934

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C 8.4010940 -5.9294365 0.0000000
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C 5.8134981 0.9591611 6.5656244
C 5.1487762 -2.4804809 6.8023678
C 4.2250725 -2.4852694 7.6246827
C 8.9012572 -0.1023232 4.7302071
C 9.3786444 0.9884841 4.3877523
C 9.5961504 -2.4642197 3.3107832
C 10.4247027 -2.3244700 2.3907606
C 5.3126616 -4.4735842 4.7908599
C 4.2473474 -5.0497679 4.5146822
C 7.7828993 -4.6836987 3.3086487
C 7.7841825 -5.5231323 2.3982196
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C 3.1739365 0.0154735 8.8768601
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C 1.5745488 3.1279143 7.9155205
C -0.3883191 0.4857181 9.8863290
C 0.3883191 -0.4857181 9.8863290
C -1.8984957 4.2537041 7.1957536
C -1.8463628 4.8095520 6.0927112
C -4.2250725 2.4852694 7.6246827
C -5.1487762 2.4804809 6.8023678
C -3.1739365 -0.0154735 8.8768601
C -3.4991140 -1.0677704 8.3057603
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C 11.2967077 1.3969617 2.0999955
C 11.6147321 0.3545209 -1.4992320
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C 7.8677512 4.8259325 1.9561741
C 6.8097981 5.1756709 1.4101970
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C -4.2473474 5.0497679 4.5146822
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C 4.1657752 4.6693469 -3.9755301

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C 6.3661399 3.2118464 -4.9693520
C 9.3786444 0.9884841 -4.3877523
C 8.9012572 -0.1023232 -4.7302071
C 0.6839077 5.0486181 -4.8496464
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C -4.2473474 5.0497679 -4.5146822
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C -11.2967077 -1.3969617 2.0999955
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C 3.4991140 1.0677704 -8.3057603
C 3.1739365 0.0154735 -8.8768601
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C -8.9012572 0.1023232 -4.7302071
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C -6.4767040 0.0541740 -6.2930011
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C 4.2250725 -2.4852694 -7.6246827
C 5.3126616 -4.4735842 -4.7908599
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C 7.7828993 -4.6836987 -3.3086487
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C -7.4794463 -3.2766304 -4.4424051
C -6.3661399 -3.2118464 -4.9693520
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C -6.8097981 -5.1756709 1.4101970
C -9.3786444 -0.9884841 4.3877523
C -8.9012572 0.1023232 4.7302071
C -7.4794463 -3.2766304 4.4424051
C -6.3661399 -3.2118464 4.9693520
C 1.8984957 -4.2537041 -7.1957536
C 1.8463628 -4.8095520 -6.0927112

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 C -5.8134981 -0.9591611 6.5656244
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 C 1.5722200 -6.2763509 0.6197301
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 C -1.6791680 -4.6012930 5.4344963
 C -0.6839077 -5.0486181 4.8496464
 C -1.5745488 -3.1279143 7.9155205
 C -0.4941380 -3.0352046 8.5182313
 C 4.0594174 -6.3649825 2.0154232
 C 5.1385035 -6.6151960 1.4690087
 C 1.8463628 -4.8095520 6.0927112
 C 1.8984957 -4.2537041 7.1957536

2.12 γ -C₂₈₈ C_{2v} 1

288
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 C -11.4948303 2.5882481 -1.5346829
 C -7.3031138 3.6093468 4.0590866
 C -7.3111705 4.0999665 2.6966560
 C -5.7679064 1.1755147 7.9320900
 C -6.6093185 0.0000000 7.8883220
 C -6.0611568 3.6101765 4.8026474
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 C -4.4686648 -0.7245865 8.3202105
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 C -5.9616463 4.8430112 -1.9668311
 C -7.0764663 4.4097317 -2.7760254
 C -4.8357012 4.0884836 4.1798462
 C -4.8309668 4.5222207 2.7989037
 C -1.2270908 2.6031363 7.0539395
 C -1.2482815 3.5780124 5.9969657
 C 0.0000000 -1.9589540 7.4175270
 C -1.2270908 -2.6031363 7.0539395
 C 0.0000000 1.9589540 7.4175270
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 C 2.5079138 -5.1023403 1.6003384
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2.13 γ -C₂₈₈ C_{2v} 2

288

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C 4.6965277 5.4983020 -4.8134587
C 7.2850464 3.3004784 -3.7910021
C 7.1970857 2.4167337 -4.6587302
C 5.5406599 2.3501711 7.3820871
C 4.9060109 3.1431467 6.6644619
C 3.9665338 0.0000000 8.1808084
C 2.7428899 0.0000000 8.0856507
C 5.5406599 -2.3501711 7.3820871
C 4.9060109 -3.1431467 6.6644619
C 11.2577395 -2.1125648 1.9292159
C 11.5390592 -1.5048480 0.8795936
C 8.9842745 -4.1178033 1.8800434
C 8.3084482 -4.4044914 0.8837751
C 7.5753590 -4.0436666 4.5046795
C 6.3567764 -4.2825573 4.5172809
C 1.9774064 6.7010830 -4.7397936
C 1.4153244 6.7443363 -3.6304224
C 4.7367236 3.5240948 -7.0063022
C 5.3016099 2.4523112 -6.7818953
C 0.6177259 6.1326901 -7.4040021
C -0.6177259 6.1326901 -7.4040021
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C 1.4185965 2.4791844 -8.3935218
C 2.0778592 5.4124758 2.2407949
C 1.4389339 5.7233169 1.2246354
C 2.0604211 3.1908636 6.6279192
C 1.4399117 2.3754912 7.3158778
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C -0.6208804 4.5291724 4.5563685
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C 8.5379230 0.0000000 -4.0705738
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C 9.1297325 -3.2397541 -1.5568789
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C -4.0655161 5.8479078 -1.2383432
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C -5.5772334 5.2656093 1.1503088

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C -9.1043725 2.1328897 6.3581035
C -8.4715250 -1.5062578 7.2234500
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C -0.6177259 -6.1326901 -7.4040021
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C -2.8570348 -6.1148902 -1.2164695
C -8.3084482 -4.4044914 0.8837751
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C -4.9465844 -5.1962295 2.2111284
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C -2.0778592 -5.4124758 2.2407949
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C -6.3567764 -4.2825573 4.5172809
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C 0.6208804 -4.5291724 4.5563685

2.14 γ -C₂₈₈ C_{2v} 3

288

Energy (BP86/SVP) = -10963.88814563 Energy (B3LYP/SVP) = -10956.37070713

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 C -1.9272860 -10.0656290 -3.4699692
 C -4.2058741 -4.2149107 -5.9558239
 C -1.1758331 -6.1893198 -7.6568018
 C -4.8941266 -4.8995711 -4.8765532
 C -0.7309662 -7.5235084 -7.3293835
 C -1.2542304 -0.7115007 -7.7017687
 C 0.0000000 -1.4051322 -7.8427439
 C -4.2945059 -2.7793442 -6.0748532
 C 0.0000000 -5.3996747 -7.9248257
 C -1.2542304 0.7115007 -7.7017687
 C 0.0000000 1.4051322 -7.8427439
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 C -5.9744687 -2.7518127 -4.2509230
 C -5.6871558 -4.1415557 -3.9501594
 C -4.2945059 2.7793442 -6.0748532
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 C -1.1758331 6.1893198 -7.6568018
 C 0.0000000 5.3996747 -7.9248257
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 C -0.7309662 7.5235084 -7.3293835
 C 0.7309662 7.5235084 -7.3293835
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 C -8.2752747 0.7202552 -1.7041600
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 C -5.2419292 -6.4760499 0.3083742
 C -8.4311050 -1.1635159 -0.3411033
 C -6.5581828 -4.4553099 0.8831756
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 C -5.2419292 6.4760499 0.3083742
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 C -2.5604548 9.7642888 -2.2074993
 C 1.9272860 10.0656290 -3.4699692
 C 2.6542553 9.3462900 -4.5187905
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 C -1.4433028 -8.6707349 2.4198135
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 C 2.5604548 9.7642888 -2.2074993
 C 0.7269253 9.2390303 1.3133103

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C 3.6734888 8.8953791 -2.4780079
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C -2.6247588 -6.6234407 6.6586388
C -5.3506952 -1.2388881 5.7652612
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C -4.4935651 5.9331475 5.1392083
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C -4.4730775 -3.4945601 6.8092030
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C 5.3067334 0.6211919 -5.3444076
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C 7.6849043 1.4837380 -2.7032599
C 2.3926629 -5.5996299 -7.2930665
C 3.2954904 -4.9443147 -6.7454762
C 1.5070735 -8.4559803 -6.6666140
C 2.1280635 -9.0448872 -5.7611921
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C 0.6222549 6.1865124 8.0905964
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C 4.9385713 5.8332920 3.9926077
C 4.4935651 5.9331475 5.1392083
C 7.3774374 3.3975345 0.4858899
C 8.0219681 2.4136890 0.1068776
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C 6.3720296 2.4647822 3.8660378
C 6.9059474 -2.0737917 -3.4638667
C 7.6849043 -1.4837380 -2.7032599
C 6.0387352 -4.6752676 -2.6809911
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C 3.8259522 0.0000000 7.2874222
C 2.7775470 0.0000000 7.9519937
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C 6.3620610 -3.4876604 3.1584900
C 4.9173426 -2.4468054 6.3285416
C 4.4730775 -3.4945601 6.8092030
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C -1.4163209 -2.4558516 8.6454274
C -2.0104684 -3.5358773 8.5040871
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2.15 γ -C₂₈₈ D_{2h} 1

288

Energy (BP86/SVP) = -10963.67277029 Energy (B3LYP/SVP) = -10956.13791078

C 3.4091505 0.7192817 10.7610251
C 2.5638410 1.1628163 11.8501740
C 3.4091505 -0.7192817 10.7610251
C 2.5638410 -1.1628163 11.8501740
C 1.9254355 0.0000000 12.4315107
C 3.4228353 4.1359595 7.2993505
C 1.1735525 5.3786825 10.3437823
C 3.8245584 2.7452954 7.3145703
C 0.7292675 4.5344317 11.4158828
C 1.1715150 8.1044125 5.7477947
C 0.0000000 8.1034995 6.5960750
C 3.4204924 4.8542632 6.0409337
C 0.0000000 6.0881225 9.8808338
C 0.7203168 8.4780759 4.4381534
C -1.1715150 8.1044125 5.7477947
C -0.7203168 8.4780759 4.4381534
C 0.7292675 -4.5344317 11.4158828
C 1.1735525 -5.3786825 10.3437823
C -0.7292675 -4.5344317 11.4158828
C 0.0000000 -6.0881225 9.8808338
C -1.1735525 -5.3786825 10.3437823
C 3.8245584 -2.7452954 7.3145703
C 3.4228353 -4.1359595 7.2993505
C 4.0802673 2.0318306 6.0756074
C 4.0802673 -2.0318306 6.0756074
C 3.8098384 4.1628594 4.8222901
C 4.0852892 2.7438248 4.8219337
C 3.4579136 6.0029333 1.2405917
C 2.5690315 7.1305805 1.2220402
C -1.9254355 0.0000000 12.4315107
C -2.5638410 -1.1628163 11.8501740
C 3.4204924 -4.8542632 6.0409337
C 0.0000000 -8.1034995 6.5960750
C 1.1715150 -8.1044125 5.7477947
C 4.0852892 -2.7438248 4.8219337
C 3.8098384 -4.1628594 4.8222901
C 4.4714207 0.7189247 1.2714712
C 4.4714207 -0.7189247 1.2714712
C 3.8037573 5.3688343 0.0000000
C 4.4934774 1.4143525 0.0000000
C 3.4579136 6.0029333 -1.2405917
C 2.5690315 7.1305805 -1.2220402

C 1.9428062 7.5323802 0.0000000
C -2.5638410 1.1628163 11.8501740
C -0.7292675 4.5344317 11.4158828
C -3.4091505 -0.7192817 10.7610251
C -3.4091505 0.7192817 10.7610251
C -3.4228353 -4.1359595 7.2993505
C -3.8245584 -2.7452954 7.3145703
C -1.1715150 -8.1044125 5.7477947
C -3.4204924 -4.8542632 6.0409337
C 0.7203168 -8.4780759 4.4381534
C -0.7203168 -8.4780759 4.4381534
C 3.4579136 -6.0029333 1.2405917
C 2.5690315 -7.1305805 1.2220402
C 4.4934774 -1.4143525 0.0000000
C 3.8037573 -5.3688343 0.0000000
C 4.4714207 0.7189247 -1.2714712
C 4.4714207 -0.7189247 -1.2714712
C 3.8098384 4.1628594 -4.8222901
C 4.0852892 2.7438248 -4.8219337
C 1.1715150 8.1044125 -5.7477947
C 0.7203168 8.4780759 -4.4381534
C 3.4204924 4.8542632 -6.0409337
C 0.0000000 8.1034995 -6.5960750
C -0.7203168 8.4780759 -4.4381534
C -1.1715150 8.1044125 -5.7477947
C -1.1735525 5.3786825 10.3437823
C -3.8245584 2.7452954 7.3145703
C -3.4228353 4.1359595 7.2993505
C -4.0802673 -2.0318306 6.0756074
C -4.0802673 2.0318306 6.0756074
C -3.8098384 -4.1628594 4.8222901
C -4.0852892 -2.7438248 4.8219337
C -2.5690315 -7.1305805 1.2220402
C -3.4579136 -6.0029333 1.2405917
C 1.9428062 -7.5323802 0.0000000
C -1.9428062 -7.5323802 0.0000000
C 3.4579136 -6.0029333 -1.2405917
C 2.5690315 -7.1305805 -1.2220402
C 4.0852892 -2.7438248 -4.8219337
C 3.8098384 -4.1628594 -4.8222901
C 4.0802673 2.0318306 -6.0756074
C 4.0802673 -2.0318306 -6.0756074
C 3.4228353 4.1359595 -7.2993505
C 3.8245584 2.7452954 -7.3145703
C 1.1735525 5.3786825 -10.3437823
C 0.0000000 6.0881225 -9.8808338
C -3.4204924 4.8542632 6.0409337
C -4.0852892 2.7438248 4.8219337
C -3.8098384 4.1628594 4.8222901
C -4.4714207 -0.7189247 1.2714712
C -4.4714207 0.7189247 1.2714712
C -3.8037573 -5.3688343 0.0000000
C -4.4934774 -1.4143525 0.0000000
C -2.5690315 -7.1305805 -1.2220402
C -3.4579136 -6.0029333 -1.2405917
C 0.7203168 -8.4780759 -4.4381534
C -0.7203168 -8.4780759 -4.4381534
C 3.4204924 -4.8542632 -6.0409337
C 1.1715150 -8.1044125 -5.7477947
C 3.8245584 -2.7452954 -7.3145703
C 3.4228353 -4.1359595 -7.2993505
C 3.4091505 0.7192817 -10.7610251
C 3.4091505 -0.7192817 -10.7610251
C 0.7292675 4.5344317 -11.4158828
C 2.5638410 1.1628163 -11.8501740
C -1.1735525 5.3786825 -10.3437823
C -0.7292675 4.5344317 -11.4158828
C -3.4579136 6.0029333 1.2405917

C -2.5690315 7.1305805 1.2220402
C -4.4934774 1.4143525 0.0000000
C -3.8037573 5.3688343 0.0000000
C -4.4714207 -0.7189247 -1.2714712
C -4.4714207 0.7189247 -1.2714712
C -3.8098384 -4.1628594 -4.8222901
C -4.0852892 -2.7438248 -4.8219337
C -1.1715150 -8.1044125 -5.7477947
C -3.4204924 -4.8542632 -6.0409337
C 0.0000000 -8.1034995 -6.5960750
C 1.1735525 -5.3786825 -10.3437823
C 0.0000000 -6.0881225 -9.8808338
C 2.5638410 -1.1628163 -11.8501740
C 0.7292675 -4.5344317 -11.4158828
C 1.9254355 0.0000000 -12.4315107
C -1.9428062 7.5323802 0.0000000
C -3.4579136 6.0029333 -1.2405917
C -2.5690315 7.1305805 -1.2220402
C -4.0852892 2.7438248 -4.8219337
C -3.8098384 4.1628594 -4.8222901
C -4.0802673 -2.0318306 -6.0756074
C -4.0802673 2.0318306 -6.0756074
C -3.4228353 -4.1359595 -7.2993505
C -3.8245584 -2.7452954 -7.3145703
C -1.1735525 -5.3786825 -10.3437823
C -3.4204924 4.8542632 -6.0409337
C -3.8245584 2.7452954 -7.3145703
C -3.4228353 4.1359595 -7.2993505
C -3.4091505 -0.7192817 -10.7610251
C -3.4091505 0.7192817 -10.7610251
C -0.7292675 -4.5344317 -11.4158828
C -2.5638410 -1.1628163 -11.8501740
C -2.5638410 1.1628163 -11.8501740
C -1.9254355 0.0000000 -12.4315107
C 3.7456866 1.4898527 9.6423661
C 3.8350214 2.0625186 8.5455728
C 2.1166968 2.4515462 12.0329903
C 1.5012361 3.5241718 11.9496520
C 3.7456866 -1.4898527 9.6423661
C 3.8350214 -2.0625186 8.5455728
C 2.1166968 -2.4515462 12.0329903
C 1.5012361 -3.5241718 11.9496520
C 0.6264362 0.0000000 12.9466520
C -0.6264362 0.0000000 12.9466520
C 2.8925576 4.7279500 8.4744719
C 2.2430337 5.1302313 9.4609028
C 2.2474261 7.2270115 5.9580347
C 2.9049856 6.1676748 5.9971204
C 0.0000000 7.7114503 7.8926862
C 0.0000000 7.0559383 8.9361783
C 1.4857608 8.2689542 3.3050496
C 2.1054600 7.7274684 2.3869668
C -2.2474261 7.2270115 5.9580347
C -2.9049856 6.1676748 5.9971204
C -1.4857608 8.2689542 3.3050496
C -2.1054600 7.7274684 2.3869668
C 2.2430337 -5.1302313 9.4609028
C 2.8925576 -4.7279500 8.4744719
C -1.5012361 -3.5241718 11.9496520
C -2.1166968 -2.4515462 12.0329903
C 0.0000000 -7.0559383 8.9361783
C 0.0000000 -7.7114503 7.8926862
C -2.2430337 -5.1302313 9.4609028
C -2.8925576 -4.7279500 8.4744719
C 4.2100360 0.6200854 6.0963973
C 4.2100360 -0.6200854 6.0963973
C 3.7991858 4.8536247 3.5929643
C 3.7370072 5.4016114 2.4851323

C 4.2753323 2.0480304 3.5841954
C 4.3893533 1.4446108 2.5046773
C 2.9049856 -6.1676748 5.9971204
C 2.2474261 -7.2270115 5.9580347
C 4.2753323 -2.0480304 3.5841954
C 4.3893533 -1.4446108 2.5046773
C 3.7991858 -4.8536247 3.5929643
C 3.7370072 -5.4016114 2.4851323
C 4.2773239 4.0442148 0.0000000
C 4.4406909 2.8209386 0.0000000
C 3.7370072 5.4016114 -2.4851323
C 3.7991858 4.8536247 -3.5929643
C 2.1054600 7.7274684 -2.3869668
C 1.4857608 8.2689542 -3.3050496
C 0.6221971 8.0424710 0.0000000
C -0.6221971 8.0424710 0.0000000
C -2.1166968 2.4515462 12.0329903
C -1.5012361 3.5241718 11.9496520
C -3.7456866 -1.4898527 9.6423661
C -3.8350214 -2.0625186 8.5455728
C -3.7456866 1.4898527 9.6423661
C -3.8350214 2.0625186 8.5455728
C -2.2474261 -7.2270115 5.9580347
C -2.9049856 -6.1676748 5.9971204
C 1.4857608 -8.2689542 3.3050496
C 2.1054600 -7.7274684 2.3869668
C -1.4857608 -8.2689542 3.3050496
C -2.1054600 -7.7274684 2.3869668
C 4.4406909 -2.8209386 0.0000000
C 4.2773239 -4.0442148 0.0000000
C 4.3893533 1.4446108 -2.5046773
C 4.2753323 2.0480304 -3.5841954
C 4.3893533 -1.4446108 -2.5046773
C 4.2753323 -2.0480304 -3.5841954
C 2.2474261 7.2270115 -5.9580347
C 2.9049856 6.1676748 -5.9971204
C 0.0000000 7.7114503 -7.8926862
C 0.0000000 7.0559383 -8.9361783
C -1.4857608 8.2689542 -3.3050496
C -2.1054600 7.7274684 -2.3869668
C -2.2474261 7.2270115 -5.9580347
C -2.9049856 6.1676748 -5.9971204
C -2.2430337 5.1302313 9.4609028
C -2.8925576 4.7279500 8.4744719
C -4.2100360 -0.6200854 6.0963973
C -4.2100360 0.6200854 6.0963973
C -3.7991858 -4.8536247 3.5929643
C -3.7370072 -5.4016114 2.4851323
C -4.2753323 -2.0480304 3.5841954
C -4.3893533 -1.4446108 2.5046773
C 0.6221971 -8.0424710 0.0000000
C -0.6221971 -8.0424710 0.0000000
C 3.7370072 -5.4016114 -2.4851323
C 3.7991858 -4.8536247 -3.5929643
C 2.1054600 -7.7274684 -2.3869668
C 1.4857608 -8.2689542 -3.3050496
C 4.2100360 0.6200854 -6.0963973
C 4.2100360 -0.6200854 -6.0963973
C 2.8925576 4.7279500 -8.4744719
C 2.2430337 5.1302313 -9.4609028
C 3.8350214 2.0625186 -8.5455728
C 3.7456866 1.4898527 -9.6423661
C -4.2753323 2.0480304 3.5841954
C -4.3893533 1.4446108 2.5046773
C -3.7991858 4.8536247 3.5929643
C -3.7370072 5.4016114 2.4851323
C -4.2773239 -4.0442148 0.0000000
C -4.4406909 -2.8209386 0.0000000

C -2.1054600 -7.7274684 -2.3869668
 C -1.4857608 -8.2689542 -3.3050496
 C -3.7370072 -5.4016114 -2.4851323
 C -3.7991858 -4.8536247 -3.5929643
 C 2.9049856 -6.1676748 -5.9971204
 C 2.2474261 -7.2270115 -5.9580347
 C 3.8350214 -2.0625186 -8.5455728
 C 3.7456866 -1.4898527 -9.6423661
 C 2.8925576 -4.7279500 -8.4744719
 C 2.2430337 -5.1302313 -9.4609028
 C 1.5012361 3.5241718 -11.9496520
 C 2.1166968 2.4515462 -12.0329903
 C -2.2430337 5.1302313 -9.4609028
 C -2.8925576 4.7279500 -8.4744719
 C -1.5012361 3.5241718 -11.9496520
 C -2.1166968 2.4515462 -12.0329903
 C -4.4406909 2.8209386 0.0000000
 C -4.2773239 4.0442148 0.0000000
 C -4.3893533 -1.4446108 -2.5046773
 C -4.2753323 -2.0480304 -3.5841954
 C -4.3893533 1.4446108 -2.5046773
 C -4.2753323 2.0480304 -3.5841954
 C -2.2474261 -7.2270115 -5.9580347
 C -2.9049856 -6.1676748 -5.9971204
 C 0.0000000 -7.7114503 -7.8926862
 C 0.0000000 -7.0559383 -8.9361783
 C 2.1166968 -2.4515462 -12.0329903
 C 1.5012361 -3.5241718 -11.9496520
 C 0.6264362 0.0000000 -12.9466520
 C -0.6264362 0.0000000 -12.9466520
 C -3.7370072 5.4016114 -2.4851323
 C -3.7991858 4.8536247 -3.5929643
 C -4.2100360 -0.6200854 -6.0963973
 C -4.2100360 0.6200854 -6.0963973
 C -2.8925576 -4.7279500 -8.4744719
 C -2.2430337 -5.1302313 -9.4609028
 C -3.8350214 -2.0625186 -8.5455728
 C -3.7456866 -1.4898527 -9.6423661
 C -3.8350214 2.0625186 -8.5455728
 C -3.7456866 1.4898527 -9.6423661
 C -1.5012361 -3.5241718 -11.9496520
 C -2.1166968 -2.4515462 -12.0329903

2.16 γ -C₂₈₈ D_{2h} 2

288

Energy (BP86/SVP) = -10963.87128630 Energy (B3LYP/SVP) = -10956.35560206

C 4.4841806 0.7323219 10.4677439
 C 4.4841806 -0.7323219 10.4677439
 C 1.1772355 2.6119061 11.2893864
 C 1.1772355 -2.6119061 11.2893864
 C 0.0000000 -1.9349386 11.8166062
 C 0.0000000 1.9349386 11.8166062
 C 5.2097040 1.1712337 9.3087320
 C 5.2097040 -1.1712337 9.3087320
 C 5.7024469 0.0000000 8.6291416
 C 4.0364585 4.0603499 6.8356688
 C 2.7288585 4.6510944 7.0421458
 C 0.7243496 3.6156073 10.3542395
 C 0.7243496 -3.6156073 10.3542395
 C -0.7243496 -3.6156073 10.3542395
 C -1.1772355 -2.6119061 11.2893864
 C 4.0364585 -4.0603499 6.8356688
 C 2.7288585 -4.6510944 7.0421458
 C 4.6571679 -4.1594183 5.535577
 C 2.0142795 -5.2441487 5.9353012
 C 4.0537386 -5.0221847 4.5612776

C 2.6864055 -5.4662379 4.6907307
C 6.8746628 0.0000000 4.7862050
C 7.0031925 -1.2492249 4.0883019
C 4.6571679 4.1594183 5.5535577
C 7.0031925 1.2492249 4.0883019
C 4.0537386 5.0221847 4.5612776
C 2.0142795 5.2441487 5.9353012
C 2.6864055 5.4662379 4.6907307
C -2.0142795 -5.2441487 5.9353012
C -2.7288585 -4.6510944 7.0421458
C 7.4801794 -1.2460567 2.7295231
C 6.0548152 -5.5617998 1.1604869
C 7.0817341 -4.6479591 0.7155876
C 7.4801794 1.2460567 2.7295231
C 7.6939981 0.0000000 2.0300994
C 7.0817341 4.6479591 0.7155876
C 6.0548152 5.5617998 1.1604869
C -2.6864055 -5.4662379 4.6907307
C -4.0364585 -4.0603499 6.8356688
C -4.0537386 -5.0221847 4.5612776
C -4.6571679 -4.1594183 5.5535577
C 0.7169941 -6.4384937 1.2625132
C -0.7169941 -6.4384937 1.2625132
C 5.3894100 6.0945596 0.0000000
C 1.4264075 -6.5279088 0.0000000
C 7.0817341 -4.6479591 -0.7155876
C 6.0548152 -5.5617998 -1.1604869
C 7.6939981 0.0000000 -2.0300994
C 7.4801794 -1.2460567 -2.7295231
C 7.0817341 4.6479591 -0.7155876
C 7.4801794 1.2460567 -2.7295231
C 5.3894100 6.0945596 0.0000000
C 6.0548152 5.5617998 -1.1604869
C -1.1772355 2.6119061 11.2893864
C -0.7243496 3.6156073 10.3542395
C -4.4841806 -0.7323219 10.4677439
C -4.4841806 0.7323219 10.4677439
C -5.2097040 -1.1712337 9.3087320
C -1.4264075 -6.5279088 0.0000000
C -6.0548152 -5.5617998 1.1604869
C -5.3894100 -6.0945596 0.0000000
C 0.7169941 -6.4384937 -1.2625132
C -0.7169941 -6.4384937 -1.2625132
C 4.0537386 -5.0221847 -4.5612776
C 2.6864055 -5.4662379 -4.6907307
C 7.0031925 -1.2492249 -4.0883019
C 4.6571679 -4.1594183 -5.5535577
C 6.8746628 0.0000000 -4.7862050
C 7.0031925 1.2492249 -4.0883019
C -5.7024469 0.0000000 8.6291416
C -5.2097040 1.1712337 9.3087320
C -7.0031925 -1.2492249 4.0883019
C -6.8746628 0.0000000 4.7862050
C -7.0817341 -4.6479591 0.7155876
C -7.4801794 -1.2460567 2.7295231
C -6.0548152 -5.5617998 -1.1604869
C -7.0817341 -4.6479591 -0.7155876
C -2.6864055 -5.4662379 -4.6907307
C -4.0537386 -5.0221847 -4.5612776
C 2.0142795 -5.2441487 -5.9353012
C -2.0142795 -5.2441487 -5.9353012
C 4.0364585 -4.0603499 -6.8356688
C 2.7288585 -4.6510944 -7.0421458
C 5.2097040 -1.1712337 -9.3087320
C 5.7024469 0.0000000 -8.6291416
C -4.0364585 4.0603499 6.8356688
C -2.7288585 4.6510944 7.0421458
C -7.0031925 1.2492249 4.0883019

C -4.6571679 4.1594183 5.5535577
C -7.6939981 0.0000000 2.0300994
C -7.4801794 1.2460567 2.7295231
C -7.4801794 -1.2460567 -2.7295231
C -7.6939981 0.0000000 -2.0300994
C -4.6571679 -4.1594183 -5.5535577
C -7.0031925 -1.2492249 -4.0883019
C -2.7288585 -4.6510944 -7.0421458
C -4.0364585 -4.0603499 -6.8356688
C 0.7243496 -3.6156073 -10.3542395
C -0.7243496 -3.6156073 -10.3542395
C 4.4841806 -0.7323219 -10.4677439
C 1.1772355 -2.6119061 -11.2893864
C 4.4841806 0.7323219 -10.4677439
C 5.2097040 1.1712337 -9.3087320
C -4.0537386 5.0221847 4.5612776
C -2.6864055 5.4662379 4.6907307
C -2.0142795 5.2441487 5.9353012
C -7.0817341 4.6479591 0.7155876
C -6.0548152 5.5617998 1.1604869
C -7.4801794 1.2460567 -2.7295231
C -7.0817341 4.6479591 -0.7155876
C -6.8746628 0.0000000 -4.7862050
C -7.0031925 1.2492249 -4.0883019
C -5.2097040 -1.1712337 -9.3087320
C -5.7024469 0.0000000 -8.6291416
C -1.1772355 -2.6119061 -11.2893864
C -4.4841806 -0.7323219 -10.4677439
C 0.0000000 -1.9349386 -11.8166062
C -6.0548152 5.5617998 -1.1604869
C -5.3894100 6.0945596 0.0000000
C -4.6571679 4.1594183 -5.5535577
C -4.0537386 5.0221847 -4.5612776
C -5.2097040 1.1712337 -9.3087320
C -4.0364585 4.0603499 -6.8356688
C -4.4841806 0.7323219 -10.4677439
C 0.0000000 1.9349386 -11.8166062
C -1.1772355 2.6119061 -11.2893864
C 1.1772355 2.6119061 -11.2893864
C -1.4264075 6.5279088 0.0000000
C -0.7169941 6.4384937 1.2625132
C -2.6864055 5.4662379 -4.6907307
C -0.7169941 6.4384937 -1.2625132
C -2.7288585 4.6510944 -7.0421458
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C 6.5153142 0.0000000 6.1395160

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2.17 γ -C₂₈₈ D_{6d} 1

288
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C 5.7938444 -3.7716208 -5.4524491
C 6.1295604 -3.2103806 -6.5067468
C -2.1442857 -5.6147621 -9.0458239
C -0.9503752 -5.9346695 -9.0458239
C -2.8865137 -2.8865137 -10.1294047
C -2.0254158 -2.0254158 -10.4124187

C -0.2919468 6.5081083 0.5441354
 C 0.2919468 6.5081083 -0.5441354
 C 5.1469998 4.2707999 -3.0305682
 C 4.2707999 5.1469998 -3.0305682
 C 6.9034269 0.3693973 -5.4524491
 C 6.9135453 -0.2845090 -6.5067468
 C 6.1632417 3.1318060 -5.4524491
 C 5.8450514 3.7031647 -6.5067468
 C 3.7903838 -4.6643869 -9.0458239
 C 4.6643869 -3.7903838 -9.0458239
 C 1.0565373 -3.9430511 -10.1294047
 C 0.7413536 -2.7667694 -10.4124187
 C 3.1318060 6.1632417 -5.4524491
 C 3.7031647 5.8450514 -6.5067468
 C 5.9346695 0.9503752 -9.0458239
 C 5.6147621 2.1442857 -9.0458239
 C 3.9430511 -1.0565373 -10.1294047
 C 2.7667694 -0.7413536 -10.4124187
 C 2.8865137 2.8865137 -10.1294047
 C 2.0254158 2.0254158 -10.4124187

2.18 γ -C₂₈₈ D_{6d} 2

288

Energy (BP86/SVP) = -10963.55558784 Energy (B3LYP/SVP) = -10956.01330156

C 9.9044150 -3.3915296 2.1593107
 C 10.2493521 -3.9339572 0.8562326
 C 10.2732398 -2.0150567 2.1593107
 C 10.8431779 -1.7177692 0.8562326
 C 10.5617431 -2.8300105 -0.0176235
 C 5.8774459 -5.8774459 2.9725819
 C 7.7317326 -7.7317326 0.0176235
 C 6.2806556 -4.5257761 3.2916581
 C 8.5315830 -6.9092207 -0.8562326
 C 3.3915296 -9.9044150 2.1593107
 C 3.9339572 -10.2493521 0.8562326
 C 4.5257761 -6.2806556 3.2916581
 C 6.9092207 -8.5315830 -0.8562326
 C 2.0150567 -10.2732398 2.1593107
 C 1.7177692 -10.8431779 0.8562326
 C 2.8300105 -10.5617431 -0.0176235
 C 10.5617431 2.8300105 0.0176235
 C 10.8431779 1.7177692 -0.8562326
 C 10.2493521 3.9339572 -0.8562326
 C 10.2732398 2.0150567 -2.1593107
 C 9.9044150 3.3915296 -2.1593107
 C 7.7020954 0.7791093 3.2916581
 C 8.0287404 2.1512945 2.9725819
 C 5.2904489 -3.5253649 3.6333485
 C 6.3443456 0.4078311 3.6333485
 C 3.5253649 -5.2904489 3.6333485
 C 3.9015416 -3.9015416 3.7430626
 C -0.7791093 -7.7020954 3.2916581
 C -0.4078311 -6.3443456 3.6333485
 C -2.8300105 -10.5617431 0.0176235
 C -1.7177692 -10.8431779 -0.8562326
 C -2.1512945 -8.0287404 2.9725819
 C -3.9339572 -10.2493521 -0.8562326
 C -3.3915296 -9.9044150 -2.1593107
 C -2.0150567 -10.2732398 -2.1593107
 C 7.0597649 3.1763192 3.2916581
 C 7.8893583 6.8817102 2.1593107
 C 8.5315830 6.9092207 0.8562326
 C 5.3296049 1.4280633 3.7430626
 C 5.6982800 2.8189807 3.6333485
 C 1.0205967 -1.0205967 3.9993207
 C 1.3941611 0.3735643 3.9993207

C -1.4280633 -5.3296049 3.7430626
C -0.3735643 -1.3941611 3.9993207
C -3.1763192 -7.0597649 3.2916581
C -2.8189807 -5.6982800 3.6333485
C -6.8817102 -7.8893583 2.1593107
C -6.9092207 -8.5315830 0.8562326
C 6.8817102 7.8893583 2.1593107
C 6.9092207 8.5315830 0.8562326
C 7.7317326 7.7317326 -0.0176235
C 2.8189807 5.6982800 3.6333485
C 3.1763192 7.0597649 3.2916581
C 0.3735643 1.3941611 3.9993207
C 1.4280633 5.3296049 3.7430626
C -1.3941611 -0.3735643 3.9993207
C -1.0205967 1.0205967 3.9993207
C -5.6982800 -2.8189807 3.6333485
C -5.3296049 -1.4280633 3.7430626
C -7.8893583 -6.8817102 2.1593107
C -7.0597649 -3.1763192 3.2916581
C -8.5315830 -6.9092207 0.8562326
C -7.7317326 -7.7317326 -0.0176235
C 2.1512945 8.0287404 2.9725819
C 2.8300105 10.5617431 0.0176235
C 3.9339572 10.2493521 -0.8562326
C 0.4078311 6.3443456 3.6333485
C 0.7791093 7.7020954 3.2916581
C -3.9015416 3.9015416 3.7430626
C -3.5253649 5.2904489 3.6333485
C -6.3443456 -0.4078311 3.6333485
C -5.2904489 3.5253649 3.6333485
C -8.0287404 -2.1512945 2.9725819
C -7.7020954 -0.7791093 3.2916581
C -10.5617431 -2.8300105 0.0176235
C -10.2493521 -3.9339572 -0.8562326
C 1.7177692 10.8431779 -0.8562326
C 2.0150567 10.2732398 -2.1593107
C 3.3915296 9.9044150 -2.1593107
C -2.0150567 10.2732398 2.1593107
C -1.7177692 10.8431779 0.8562326
C -4.5257761 6.2806556 3.2916581
C -3.3915296 9.9044150 2.1593107
C -6.2806556 4.5257761 3.2916581
C -5.8774459 5.8774459 2.9725819
C -10.2732398 2.0150567 2.1593107
C -9.9044150 3.3915296 2.1593107
C -10.8431779 -1.7177692 -0.8562326
C -10.8431779 1.7177692 0.8562326
C -9.9044150 -3.3915296 -2.1593107
C -10.2732398 -2.0150567 -2.1593107
C -5.8774459 -5.8774459 -2.9725819
C -6.2806556 -4.5257761 -3.2916581
C -4.5257761 -6.2806556 -3.2916581
C -3.9339572 10.2493521 0.8562326
C -2.8300105 10.5617431 -0.0176235
C -7.7317326 7.7317326 0.0176235
C -6.9092207 8.5315830 -0.8562326
C -10.2493521 3.9339572 0.8562326
C -8.5315830 6.9092207 -0.8562326
C -10.5617431 2.8300105 -0.0176235
C -7.7020954 0.7791093 -3.2916581
C -8.0287404 2.1512945 -2.9725819
C -5.2904489 -3.5253649 -3.6333485
C -6.3443456 0.4078311 -3.6333485
C -3.5253649 -5.2904489 -3.6333485
C -3.9015416 -3.9015416 -3.7430626
C 0.7791093 -7.7020954 -3.2916581
C 0.4078311 -6.3443456 -3.6333485
C 2.1512945 -8.0287404 -2.9725819

C -7.0597649 3.1763192 -3.2916581
C -7.8893583 6.8817102 -2.1593107
C -5.3296049 1.4280633 -3.7430626
C -5.6982800 2.8189807 -3.6333485
C -1.0205967 -1.0205967 -3.9993207
C -1.3941611 0.3735643 -3.9993207
C 1.4280633 -5.3296049 -3.7430626
C 0.3735643 -1.3941611 -3.9993207
C 3.1763192 -7.0597649 -3.2916581
C 2.8189807 -5.6982800 -3.6333485
C 6.8817102 -7.8893583 -2.1593107
C -6.8817102 7.8893583 -2.1593107
C -2.8189807 5.6982800 -3.6333485
C -3.1763192 7.0597649 -3.2916581
C -0.3735643 1.3941611 -3.9993207
C -1.4280633 5.3296049 -3.7430626
C 1.3941611 -0.3735643 -3.9993207
C 1.0205967 1.0205967 -3.9993207
C 5.6982800 -2.8189807 -3.6333485
C 5.3296049 -1.4280633 -3.7430626
C 7.8893583 -6.8817102 -2.1593107
C 7.0597649 -3.1763192 -3.2916581
C -2.1512945 8.0287404 -2.9725819
C -0.4078311 6.3443456 -3.6333485
C -0.7791093 7.7020954 -3.2916581
C 3.9015416 3.9015416 -3.7430626
C 3.5253649 5.2904489 -3.6333485
C 6.3443456 -0.4078311 -3.6333485
C 5.2904489 3.5253649 -3.6333485
C 8.0287404 -2.1512945 -2.9725819
C 7.7020954 -0.7791093 -3.2916581
C 4.5257761 6.2806556 -3.2916581
C 6.2806556 4.5257761 -3.2916581
C 5.8774459 5.8774459 -2.9725819
C 8.8069144 -3.9044345 2.8576691
C 7.6301798 -4.1822717 3.1336755
C 9.9515373 -5.1640804 0.3601357
C 9.4479934 -6.0362439 -0.3601357
C 9.5792289 -1.0221178 2.8576691
C 8.6990654 -0.1931363 3.1336755
C 11.2003243 -0.5035438 0.3601357
C 11.2003243 0.5035438 -0.3601357
C 10.0225634 -2.6855378 -1.3101395
C 9.1880941 -2.4619424 -2.2148779
C 6.7261517 -6.7261517 2.2148779
C 7.3370257 -7.3370257 1.3101395
C 3.9044345 -8.8069144 2.8576691
C 4.1822717 -7.6301798 3.1336755
C 5.1640804 -9.9515373 0.3601357
C 6.0362439 -9.4479934 -0.3601357
C 1.0221178 -9.5792289 2.8576691
C 0.1931363 -8.6990654 3.1336755
C 0.5035438 -11.2003243 0.3601357
C -0.5035438 -11.2003243 -0.3601357
C 2.6855378 -10.0225634 -1.3101395
C 2.4619424 -9.1880941 -2.2148779
C 10.0225634 2.6855378 1.3101395
C 9.1880941 2.4619424 2.2148779
C 9.9515373 5.1640804 -0.3601357
C 9.4479934 6.0362439 0.3601357
C 9.5792289 1.0221178 -2.8576691
C 8.6990654 0.1931363 -3.1336755
C 8.8069144 3.9044345 -2.8576691
C 7.6301798 4.1822717 -3.1336755
C 5.6738202 -2.1623047 3.7290733
C 5.9948248 -0.9642993 3.7290733
C 2.1623047 -5.6738202 3.7290733
C 0.9642993 -5.9948248 3.7290733

C 2.9013431 -2.9013431 3.8956232
C 2.0270504 -2.0270504 3.9617112
C -2.6855378 -10.0225634 1.3101395
C -2.4619424 -9.1880941 2.2148779
C -5.1640804 -9.9515373 -0.3601357
C -6.0362439 -9.4479934 0.3601357
C -3.9044345 -8.8069144 -2.8576691
C -4.1822717 -7.6301798 -3.1336755
C -1.0221178 -9.5792289 -2.8576691
C -0.1931363 -8.6990654 -3.1336755
C 7.4370434 4.5167936 3.1336755
C 7.7847966 5.6747944 2.8576691
C 3.9633084 1.0619653 3.8956232
C 2.7690024 0.7419520 3.9617112
C 4.7095209 3.8325201 3.7290733
C 3.8325201 4.7095209 3.7290733
C -1.0619653 -3.9633084 3.8956232
C -0.7419520 -2.7690024 3.9617112
C -4.5167936 -7.4370434 3.1336755
C -5.6747944 -7.7847966 2.8576691
C -3.8325201 -4.7095209 3.7290733
C -4.7095209 -3.8325201 3.7290733
C 5.6747944 7.7847966 2.8576691
C 4.5167936 7.4370434 3.1336755
C 6.0362439 9.4479934 0.3601357
C 5.1640804 9.9515373 -0.3601357
C 7.3370257 7.3370257 -1.3101395
C 6.7261517 6.7261517 -2.2148779
C 0.7419520 2.7690024 3.9617112
C 1.0619653 3.9633084 3.8956232
C -2.7690024 -0.7419520 3.9617112
C -3.9633084 -1.0619653 3.8956232
C -2.0270504 2.0270504 3.9617112
C -2.9013431 2.9013431 3.8956232
C -7.7847966 -5.6747944 2.8576691
C -7.4370434 -4.5167936 3.1336755
C -9.4479934 -6.0362439 0.3601357
C -9.9515373 -5.1640804 -0.3601357
C -7.3370257 -7.3370257 -1.3101395
C -6.7261517 -6.7261517 -2.2148779
C 2.4619424 9.1880941 2.2148779
C 2.6855378 10.0225634 1.3101395
C -0.9642993 5.9948248 3.7290733
C -2.1623047 5.6738202 3.7290733
C -0.1931363 8.6990654 3.1336755
C -1.0221178 9.5792289 2.8576691
C -5.9948248 0.9642993 3.7290733
C -5.6738202 2.1623047 3.7290733
C -9.1880941 -2.4619424 2.2148779
C -10.0225634 -2.6855378 1.3101395
C -8.6990654 0.1931363 3.1336755
C -9.5792289 1.0221178 2.8576691
C 0.5035438 11.2003243 -0.3601357
C -0.5035438 11.2003243 0.3601357
C 1.0221178 9.5792289 -2.8576691
C 0.1931363 8.6990654 -3.1336755
C 3.9044345 8.8069144 -2.8576691
C 4.1822717 7.6301798 -3.1336755
C -4.1822717 7.6301798 3.1336755
C -3.9044345 8.8069144 2.8576691
C -7.6301798 4.1822717 3.1336755
C -8.8069144 3.9044345 2.8576691
C -6.7261517 6.7261517 2.2148779
C -7.3370257 7.3370257 1.3101395
C -11.2003243 -0.5035438 -0.3601357
C -11.2003243 0.5035438 0.3601357
C -8.8069144 -3.9044345 -2.8576691
C -7.6301798 -4.1822717 -3.1336755

C -9.5792289 -1.0221178 -2.8576691
 C -8.6990654 -0.1931363 -3.1336755
 C -5.1640804 9.9515373 0.3601357
 C -6.0362439 9.4479934 -0.3601357
 C -2.6855378 10.0225634 -1.3101395
 C -2.4619424 9.1880941 -2.2148779
 C -9.9515373 5.1640804 0.3601357
 C -9.4479934 6.0362439 -0.3601357
 C -10.0225634 2.6855378 -1.3101395
 C -9.1880941 2.4619424 -2.2148779
 C -5.6738202 -2.1623047 -3.7290733
 C -5.9948248 -0.9642993 -3.7290733
 C -2.1623047 -5.6738202 -3.7290733
 C -0.9642993 -5.9948248 -3.7290733
 C -2.9013431 -2.9013431 -3.8956232
 C -2.0270504 -2.0270504 -3.9617112
 C -7.4370434 4.5167936 -3.1336755
 C -7.7847966 5.6747944 -2.8576691
 C -3.9633084 1.0619653 -3.8956232
 C -2.7690024 0.7419520 -3.9617112
 C -4.7095209 3.8325201 -3.7290733
 C -3.8325201 4.7095209 -3.7290733
 C 1.0619653 -3.9633084 -3.8956232
 C 0.7419520 -2.7690024 -3.9617112
 C 4.5167936 -7.4370434 -3.1336755
 C 5.6747944 -7.7847966 -2.8576691
 C 3.8325201 -4.7095209 -3.7290733
 C 4.7095209 -3.8325201 -3.7290733
 C -5.6747944 7.7847966 -2.8576691
 C -4.5167936 7.4370434 -3.1336755
 C -0.7419520 2.7690024 -3.9617112
 C -1.0619653 3.9633084 -3.8956232
 C 2.7690024 -0.7419520 -3.9617112
 C 3.9633084 -1.0619653 -3.8956232
 C 2.0270504 2.0270504 -3.9617112
 C 2.9013431 2.9013431 -3.8956232
 C 7.7847966 -5.6747944 -2.8576691
 C 7.4370434 -4.5167936 -3.1336755
 C 0.9642993 5.9948248 -3.7290733
 C 2.1623047 5.6738202 -3.7290733
 C 5.9948248 0.9642993 -3.7290733
 C 5.6738202 2.1623047 -3.7290733

2.19 γ -C₄₃₂

432

Energy (BP86/SVP) = -16445.71398162 Energy (B3LYP/SVP) = -16434.46360674

C 4.0619790 -1.2494550 9.9524700
 C 3.7391355 0.0000000 10.6124270
 C 1.2494550 -4.0619790 9.9524700
 C 0.0000000 -3.7391355 10.6124270
 C -0.0000000 -1.0386908 13.4836745
 C 1.0386908 -0.0000000 13.4836745
 C 4.9995385 -1.2481808 8.8763653
 C 5.554535 -0.0000000 8.4109957
 C 4.9995385 1.2481808 8.8763653
 C 4.0619790 1.2494550 9.9524700
 C 1.2481808 -4.9995385 8.8763653
 C -0.0000000 -5.554535 8.4109957
 C -1.2481808 -4.9995385 8.8763653
 C -1.2494550 -4.0619790 9.9524700
 C 5.5291671 -4.5110114 6.5393301
 C 4.5110114 -5.5291671 6.5393301
 C 8.8763653 -1.2481808 4.9995385
 C 8.4109957 0.0000000 5.554535
 C 6.5393301 -4.5110114 5.5291671
 C 9.9524700 -1.2494550 4.0619790

C 10.6124270 -0.0000000 3.7391355
C 9.9524700 1.2494550 4.0619790
C 8.8763653 1.2481808 4.9995385
C 4.5110114 -6.5393301 5.5291671
C 1.2481808 -8.8763653 4.9995385
C 0.0000000 -8.4109957 5.5554535
C 6.5393301 -5.5291671 4.5110114
C 5.5291671 -6.5393301 4.5110114
C 9.9524700 -4.0619790 1.2494550
C 8.8763653 -4.9995385 1.2481808
C 13.4836745 -1.0386908 0.0000000
C 13.4836745 0.0000000 1.0386908
C 10.6124270 -3.7391355 0.0000000
C 13.4836745 0.0000000 -1.0386908
C 13.4836745 1.0386908 -0.0000000
C 1.2494550 -9.9524700 4.0619790
C -0.0000000 -10.6124270 3.7391355
C -1.2494550 -9.9524700 4.0619790
C -1.2481808 -8.8763653 4.9995385
C 4.9995385 -8.8763653 1.2481808
C 4.0619790 -9.9524700 1.2494550
C 8.4109957 -5.5554535 -0.0000000
C 5.5554535 -8.4109957 -0.0000000
C 9.9524700 -4.0619790 -1.2494550
C 8.8763653 -4.9995385 -1.2481808
C 9.9524700 -1.2494550 -4.0619790
C 10.6124270 -0.0000000 -3.7391355
C 3.7391355 -10.6124270 0.0000000
C 1.0386908 -13.4836745 0.0000000
C 0.0000000 -13.4836745 1.0386908
C 4.9995385 -8.8763653 -1.2481808
C 4.0619790 -9.9524700 -1.2494550
C 6.5393301 -5.5291671 -4.5110114
C 5.5291671 -6.5393301 -4.5110114
C 8.8763653 -1.2481808 -4.9995385
C 6.5393301 -4.5110114 -5.5291671
C 8.4109957 0.0000000 -5.5554535
C 8.8763653 1.2481808 -4.9995385
C 9.9524700 1.2494550 -4.0619790
C 0.0000000 -13.4836745 -1.0386908
C -1.0386908 -13.4836745 -0.0000000
C 1.2494550 -9.9524700 -4.0619790
C -0.0000000 -10.6124270 -3.7391355
C 4.5110114 -6.5393301 -5.5291671
C 1.2481808 -8.8763653 -4.9995385
C 5.5291671 -4.5110114 -6.5393301
C 4.5110114 -5.5291671 -6.5393301
C 4.9995385 -1.2481808 -8.8763653
C 5.5554535 -0.0000000 -8.4109957
C -3.7391355 -10.6124270 0.0000000
C -4.0619790 -9.9524700 1.2494550
C -1.2494550 -9.9524700 -4.0619790
C -4.0619790 -9.9524700 -1.2494550
C 0.0000000 -8.4109957 -5.5554535
C -1.2481808 -8.8763653 -4.9995385
C 1.2481808 -4.9995385 -8.8763653
C -0.0000000 -5.5554535 -8.4109957
C 4.0619790 -1.2494550 -9.9524700
C 1.2494550 -4.0619790 -9.9524700
C 3.7391355 0.0000000 -10.6124270
C 4.0619790 1.2494550 -9.9524700
C 4.9995385 1.2481808 -8.8763653
C -4.5110114 -6.5393301 5.5291671
C -4.5110114 -5.5291671 6.5393301
C -4.9995385 -8.8763653 1.2481808
C -5.5291671 -6.5393301 4.5110114
C -4.9995385 -8.8763653 -1.2481808
C -5.5554535 -8.4109957 0.0000000

C -4.5110114 -6.5393301 -5.5291671
C -5.5291671 -6.5393301 -4.5110114
C -1.2481808 -4.9995385 -8.8763653
C -4.5110114 -5.5291671 -6.5393301
C 0.0000000 -3.7391355 -10.6124270
C -1.2494550 -4.0619790 -9.9524700
C -0.0000000 -1.0386908 -13.4836745
C 1.0386908 -0.0000000 -13.4836745
C -1.0386908 0.0000000 13.4836745
C 0.0000000 1.0386908 13.4836745
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2.20 γ -C₆₄₈

648

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C 18.3534969 0.0000000 -1.0656657
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2.21 β -C₆₄₈

648

Energy (BP86/SVP) = -24664.56418022 Energy (B3LYP/SVP) = -24647.73109680

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 C 3.4399232 -4.4741495 14.0520135
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 C 2.7493074 0.0000000 16.9593751
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 C 9.1264982 0.0000000 10.1649463
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 C -3.4399232 -4.4741495 14.0520135
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 C 4.6260143 -7.4780127 10.3267980

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2.22 β -C₇₂@C₂₁₆

288

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936

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120

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C -1.1955735 -5.9248856 -3.8849711
C -2.1642579 -6.0918328 -3.1171868

C -3.1171868 -6.0918328 -2.1642579
 C -3.8849711 -5.9248856 -1.1955735
 C -1.1955735 -3.8849711 -5.9248856
 C -2.1642579 -3.1171868 -6.0918328
 C -3.1171868 -2.1642579 -6.0918328
 C -3.8849711 -1.1955735 -5.9248856
 C -5.9248856 -3.8849711 -1.1955735
 C -6.0918328 -3.1171868 -2.1642579
 C -6.0918328 -2.1642579 -3.1171868
 C -5.9248856 -1.1955735 -3.8849711
 C -5.9248856 -3.8849711 1.1955735
 C -6.0918328 -3.1171868 2.1642579
 C -6.0918328 -2.1642579 3.1171868
 C -5.9248856 -1.1955735 3.8849711
 C -5.9248856 1.1955735 -3.8849711
 C -6.0918328 2.1642579 -3.1171868
 C -6.0918328 3.1171868 -2.1642579
 C -5.9248856 3.8849711 -1.1955735
 C -5.9248856 1.1955735 3.8849711
 C -6.0918328 2.1642579 3.1171868
 C -6.0918328 3.1171868 2.1642579
 C -5.9248856 3.8849711 1.1955735

2.25 β -C₄-C₃₆₀

360

Energy (BP86/SVP) = -13701.50227419 Energy (B3LYP/SVP) = -13692.25136306

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 C -3.2235752 -3.2235752 -12.6492560
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 C -0.7237742 -8.9585391 -8.9585391
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 C -4.0705815 -4.0705815 -11.8352498
 C 3.2235752 -12.6492560 -3.2235752
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 C -4.0705815 -11.8352498 -4.0705815
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 C -3.2235752 -12.6492560 3.2235752
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 C 8.9585391 0.7237742 -8.9585391
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 C 8.9585391 -8.9585391 -0.7237742
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 C 4.0705815 -11.8352498 4.0705815
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 C -0.7237742 -8.9585391 8.9585391
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 C 4.0705815 -4.0705815 11.8352498
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C -12.6492560 -3.2235752 -3.2235752
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C 1.4603245 -8.0611963 -9.7491059
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 C -10.3365829 2.1826052 -7.2304990
 C -9.7491059 1.4603245 -8.0611963

2.26 γ -C₄-C₁₀₈

108

Energy (BP86/SVP) = -4110.351259632 Energy (B3LYP/SVP) = -4107.482950555

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 C 7.4451013 0.0000000 1.0275372
 C 7.6582906 1.0452010 -0.0000000
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 C 3.7225507 -6.4476469 -1.0275372
 C 4.7343159 -6.1096737 -0.0000000
 C 1.4651583 0.0000000 -3.2836325
 C -2.9239747 -7.1548747 -0.0000000
 C -3.7225507 -6.4476469 -1.0275372
 C 2.9239747 -7.1548747 0.0000000
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 C -3.7225507 -6.4476469 1.0275372
 C -4.7343159 -6.1096737 0.0000000

C 0.7325791 -1.2688643 3.2836325
C 3.7225507 -6.4476469 1.0275372
C -0.7325791 -1.2688643 3.2836325
C 1.4651583 0.0000000 3.2836325
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