Electronic Supplementary Information (ESI)

Multistructural partition function truncation and its effect on the thermal rate constants

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S.1.   Nomenclature IUPAC - Dihedral Angles

- C $\Rightarrow \phi_i = 0°$

- C$-$ $\Rightarrow \phi_i \in (-30°, 0°) \Leftrightarrow$ C$+$ $\Rightarrow \phi_i \in (0°, +30°)$;

- G$-$ $\Rightarrow \phi_i \in (-75°, -30°) \Leftrightarrow$ G$+$ $\Rightarrow \phi_i \in (+30°, +75°)$;

- g$-$ $\Rightarrow \phi_i \in (-90°, -75°) \Leftrightarrow$ g$+$ $\Rightarrow \phi_i \in (+75°, +90°)$;

- a$-$ $\Rightarrow \phi_i \in (-105°, -90°) \Leftrightarrow$ a$+$ $\Rightarrow \phi_i \in (+90°, +105°)$;

- A$-$ $\Rightarrow \phi_i \in (-150°, -105°) \Leftrightarrow$ A$+$ $\Rightarrow \phi_i \in (+105°, +150°)$;

- T$-$ $\Rightarrow \phi_i \in (-180°, -105°) \Leftrightarrow$ T$+$ $\Rightarrow \phi_i \in (+150°, +180°)$;

- T $\Rightarrow \phi_i = 180°$.

S.2.   Cartesian Coordinates

S.2.1   Methyl Pentanoate

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* E =  +0.000 kcal/mol ; Conformer 001
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51495
C   +1.40178    +0.00000    +2.09498
C   +1.42194    +0.00408    +3.60884
C   +0.94896    -1.28765    +4.20236
O   +0.68709    -1.16555    +5.50227
C   +0.27722    -2.35483    +6.15344
O   +0.83371    -2.32715    +3.61062
H   +0.10887    -2.08365    +7.18753
H   -0.63451    -2.73719    +5.70533
H   +1.04953    -3.11400    +6.07822
H   +2.43209    +0.16382    +3.98743
H   +0.81848    +0.81171    +4.02021
H   +1.94038    -0.87667    +1.73717
H   +1.94335    +0.87522    +1.73583
H   -0.54039    +0.87471    +1.88178
H   -0.53467    -0.87612    +1.87995
H   -1.01156    +0.00502    -0.39880
H   +0.51569    +0.87454    -0.39395
H   +0.50418    -0.88294    -0.38841

* E =  +0.146 kcal/mol ; Conformer 002
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51519
C   +1.39944    +0.00000    +2.09806
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C    +1.39579    +0.00000    +3.60978
C    +2.77162    +0.00000    +4.19795
O    +2.73540    +0.00000    +5.53005
C    +3.99865    +0.00000    +6.17057
O    +3.79803    -0.00000    +3.57437
H    +3.79200    +0.00000    +7.23295
H    +4.56555    -0.88279    +5.89176
H    +4.56555    +0.88279    +5.89176
H    +0.86798    +0.86787    +4.00614
H    +0.86798    -0.86787    +4.00614
H    +1.95176    -0.86849    +1.74047
H    +1.95176    +0.86849    +1.74047
H    -0.54524    +0.87186    +1.88081
H    -0.54524    -0.87186    +1.88081
H    -1.01117    -0.00000    -0.39973
H    +0.51136    +0.87781    -0.39097
H    +0.51136    -0.87781    -0.39097

* E =   +0.687 kcal/mol ; Conformer 003
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51682
C    +1.38908    +0.00000    +2.13479
C    +2.20421    -1.24155    +1.83220
C    +1.65033    -2.47373    +2.47937
O    +2.14943    -3.58319    +1.93704
C    +1.71561    -4.79540    +2.52750
O    +0.87105    -2.49133    +3.39392
H    +2.20830    -5.58633    +1.97706
H    +1.99515    -4.82795    +3.57599
H    +0.63707    -4.88998    +2.44965
H    +2.30392    -1.42628    +0.76516
H    +3.22226    -1.13150    +2.20786
H    +1.94268    +0.86973    +1.77993
H    +1.29927    +0.09724    +3.21487
H    -0.53128    +0.88213    +1.87254
H    -0.55627    -0.85812    +1.89247
H    -1.01230    +0.07021    -0.39088
H    +0.56457    +0.84470    -0.39303
H    +0.43843    -0.90786    -0.40979

* E =   +0.728 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51684
C    +1.38712    +0.00000    +2.13553
C    +2.18792    -1.24122    +1.80713
C    +3.50759    -1.28158    +2.51149
O    +4.20743    -2.36603    +2.17983
C    +5.47113    -2.48758    +2.80735
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O    +3.91328    -0.45746    +3.28544
H    +5.90029    -3.40840    +2.43411
H    +6.10296    -1.64174    +2.55478
H    +5.35672    -2.52920    +3.88609
H    +1.64293    -2.14581    +2.08103
H    +2.38647    -1.33077    +0.74014
H    +1.93988    +0.87921    +1.80479
H    +1.30962    +0.08845    +3.21734
H    -0.53613    +0.87871    +1.87348
H    -0.55915    -0.86336    +1.88199
H    -1.01060    +0.08062    -0.39319
H    +0.57382    +0.83982    -0.38946
H    +0.43219    -0.91184    -0.40712

* E =  +0.822 kcal/mol ; Conformer 005
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51492
C    +1.40032    +0.00000    +2.09742
C    +1.41348    -0.02192    +3.61610
C    +0.75558    +1.16321    +4.25516
O    +1.07168    +2.30420    +3.64297
C    +0.51259    +3.47331    +4.21364
O    +0.04314    +1.12313    +5.22168
H    +0.85938    +4.29710    +3.60330
H    -0.57156    +3.41899    +4.20280
H    +0.84610    +3.59081    +5.24000
H    +0.91469    -0.90372    +4.00823
H    +2.44081    -0.04382    +3.98075
H    +1.94457    -0.87229    +1.73503
H    +1.94141    +0.87718    +1.74574
H    -0.53976    +0.87583    +1.87844
H    -0.54466    -0.87008    +1.88421
H    -1.01139    +0.00117    -0.39901
H    +0.51161    +0.87792    -0.39051
H    +0.50937    -0.87883    -0.39193

* E =  +0.995 kcal/mol ; Conformer 006
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51512
C    +1.39973    +0.00000    +2.09793
C    +1.39047    +0.00686    +3.61897
C    +2.76182    +0.01139    +4.21665
O    +3.48359    -1.03223    +3.80737
C    +4.79782    -1.10327    +4.32986
O    +3.19088    +0.83760    +4.97601
H    +5.23931    -1.99450    +3.90305
H    +5.36599    -0.22243    +4.04765
H    +4.77191    -1.17061    +5.41303
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H    +0.87187    +0.87938    +4.00457
H    +0.87140    -0.88049    +3.98222
H    +1.94693    -0.87389    +1.74717
H    +1.94260    +0.87416    +1.73537
H    -0.54434    +0.87121    +1.88200
H    -0.54106    -0.87351    +1.88221
H    -1.01160    -0.00200    -0.39843
H    +0.50810    +0.87949    -0.39152
H    +0.51226    -0.87704    -0.39156

* E =  +1.102 kcal/mol ; Conformer 007
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51653
C    +1.38562    +0.00000    +2.14215
C    +2.24188    -1.18554    +1.73222
C    +2.95043    -0.98237    +0.42748
O    +3.20325    -2.13716    -0.18580
C    +3.92684    -2.03315    -1.39914
O    +3.29421    +0.07899    -0.01874
H    +4.04940    -3.04648    -1.75895
H    +3.37527    -1.43591    -2.11847
H    +4.89284    -1.56906    -1.22618
H    +3.03054    -1.35525    +2.46641
H    +1.66748    -2.10861    +1.68309
H    +1.91537    +0.91290    +1.87277
H    +1.28206    +0.00012    +3.22566
H    -0.53965    +0.87540    +1.87691
H    -0.55439    -0.86790    +1.87858
H    -1.01209    +0.08505    -0.38873
H    +0.58792    +0.82637    -0.39343
H    +0.41959    -0.92158    -0.40195

* E =  +1.216 kcal/mol ; Conformer 008
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51650
C    +1.38965    +0.00000    +2.13248
C    +2.25446    -1.17658    +1.69403
C    +1.58141    -2.49124    +1.93406
O    +1.29902    -2.67362    +3.22392
C    +0.64433    -3.88966    +3.53659
O    +1.30227    -3.29849    +1.08853
H    +0.49072    -3.87763    +4.60787
H    -0.30560    -3.95385    +3.01492
H    +1.25941    -4.73635    +3.24812
H    +2.48823    -1.12819    +0.63567
H    +3.19195    -1.16772    +2.24744
H    +1.90903    +0.91985    +1.86330
H    +1.30467    -0.01063    +3.21738
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H    -0.53925    +0.87237    +1.88425
H    -0.55357    -0.86849    +1.87887
H    -1.00992    +0.09956    -0.39009
H    +0.58888    +0.82849    -0.39215
H    +0.41165    -0.92455    -0.39896


* E =  +1.556 kcal/mol ; Conformer 009
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51642
C    +1.38852    +0.00000    +2.13309
C    +2.19078    -1.24921    +1.79572
C    +3.52034    -1.28900    +2.47918
O    +4.25534    -0.21359    +2.19536
C    +5.53385    -0.17494    +2.80287
O    +3.90989    -2.16762    +3.20024
H    +5.99037    +0.75023    +2.47563
H    +5.44045    -0.19375    +3.88421
H    +6.12876    -1.02686    +2.48848
H    +1.65561    -2.14871    +2.08621
H    +2.37296    -1.29682    +0.72278
H    +1.94162    +0.87734    +1.80017
H    +1.29790    +0.08031    +3.21624
H    -0.53373    +0.87990    +1.87421
H    -0.55810    -0.86274    +1.88317
H    -1.01079    +0.08579    -0.39135
H    +0.57813    +0.83632    -0.39042
H    +0.42578    -0.91469    -0.40701


* E =  +1.593 kcal/mol ; Conformer 010
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51643
C    +1.38692    +0.00000    +2.13647
C    +2.19299    -1.24718    +1.79861
C    +3.52561    -1.27448    +2.47806
O    +3.40553    -1.25006    +3.80567
C    +4.62457    -1.27035    +4.52571
O    +4.59167    -1.31218    +1.92518
H    +4.35164    -1.24635    +5.57279
H    +5.18465    -2.17180    +4.29722
H    +5.23095    -0.40741    +4.26876
H    +1.63727    -2.13124    +2.11293
H    +2.38280    -1.32622    +0.73362
H    +1.93396    +0.88173    +1.79894
H    +1.30250    +0.07736    +3.21854
H    -0.53548    +0.87884    +1.87428
H    -0.55630    -0.86404    +1.88362
H    -1.01111    +0.08114    -0.39150
H    +0.57403    +0.83924    -0.39009
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H    +0.43167    -0.91170    -0.40703


* E  =   +1.798 kcal/mol ; Conformer 011
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51713
C    +1.38158    +0.00000    +2.15128
C    +2.20963    -1.24397    +1.86337
C    +2.77673    -1.34847    +0.48069
O    +3.27622    -0.19058    +0.05126
C    +3.85020    -0.22208    -1.24252
O    +2.82321    -2.35569    -0.17362
H    +4.21283    +0.78008    -1.43144
H    +4.66533    -0.93791    -1.27947
H    +3.10370    -0.50335    -1.97923
H    +3.06716    -1.26986    +2.53687
H    +1.64033    -2.15285    +2.03933
H    +1.93751    +0.87922    +1.82850
H    +1.26839    +0.08152    +3.23132
H    -0.53609    +0.87944    +1.87332
H    -0.56003    -0.86317    +1.88064
H    -1.01030    +0.11121    -0.38674
H    +0.59977    +0.82064    -0.39010
H    +0.39637    -0.92740    -0.40829


* E  =   +8.065 kcal/mol ; Conformer 012
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51486
C    +1.40277    +0.00000    +2.09241
C    +1.42425    +0.00179    +3.60708
C    +0.99137    +1.32241    +4.18674
O    +0.81837    +1.39566    +5.51326
C    +0.99137    +0.26856    +6.33988
O    +0.81977    +2.30767    +3.53003
H    +0.88354    +0.62924    +7.35526
H    +0.23057    -0.48546    +6.15032
H    +1.97893    -0.17142    +6.22353
H    +0.79351    -0.79573    +4.00070
H    +2.42946    -0.20207    +3.98037
H    +1.94077    -0.87952    +1.73802
H    +1.94253    +0.87412    +1.73201
H    -0.53332    +0.87552    +1.88112
H    -0.53841    -0.87679    +1.88069
H    -1.01188    -0.00852    -0.39768
H    +0.49980    +0.88561    -0.38764
H    +0.51889    -0.87220    -0.39515


* E  =   +8.144 kcal/mol ; Conformer 013
C    +0.00000    +0.00000    +0.00000
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C    +0.00000    +0.00000    +1.51519
C    +1.40035    +0.00000    +2.09568
C    +1.39970    +0.00001    +3.60806
C    +2.79105    -0.00008    +4.17813
O    +2.91985    +0.00054    +5.51247
C    +1.79319    +0.00099    +6.35702
O    +3.77904    -0.00066    +3.50407
H    +2.18268    +0.00072    +7.36744
H    +1.18323    +0.89001    +6.21373
H    +1.18239    -0.88742    +6.21359
H    +0.86269    +0.86923    +3.99194
H    +0.86266    -0.86921    +3.99190
H    +1.95427    -0.86774    +1.74062
H    +1.95427    +0.86774    +1.74059
H    -0.54531    +0.87233    +1.87992
H    -0.54531    -0.87233    +1.87992
H    -1.01130    -0.00000    -0.39930
H    +0.51143    +0.87776    -0.39057
H    +0.51143    -0.87776    -0.39057

* E =  +8.726 kcal/mol ; Conformer 014
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51692
C    +1.38606    +0.00000    +2.13747
C    +2.18656    -1.24351    +1.81458
C    +3.51701    -1.25467    +2.51519
O    +4.32002    -2.30921    +2.31396
C    +3.93646    -3.37284    +1.47497
O    +3.89052    -0.37634    +3.23601
H    +4.75905    -4.07677    +1.49732
H    +3.03817    -3.86766    +1.83714
H    +3.78271    -3.04176    +0.45037
H    +1.63173    -2.13985    +2.09926
H    +2.36125    -1.33326    +0.74211
H    +1.94404    +0.87488    +1.80601
H    +1.31045    +0.09112    +3.21875
H    -0.53409    +0.88023    +1.87247
H    -0.56255    -0.86102    +1.88273
H    -1.01004    +0.08603    -0.39327
H    +0.57832    +0.83661    -0.38947
H    +0.42634    -0.91432    -0.40849

* E =  +8.776 kcal/mol ; Conformer 015
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51683
C    +1.38890    +0.00000    +2.13532
C    +2.20276    -1.24518    +1.84109
C    +1.66728    -2.46256    +2.54641
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O   +2.20391   -3.65085   +2.23698
C   +3.21325   -3.76945   +1.26194
O   +0.81052   -2.41970   +3.38052
H   +3.52584   -4.80601   +1.28660
H   +2.83683   -3.53792   +0.26791
H   +4.06854   -3.13630   +1.48542
H   +2.26096   -1.43546   +0.77042
H   +3.23474   -1.10923   +2.16985
H   +1.94497   +0.86478   +1.77176
H   +1.30022   +0.10429   +3.21430
H   -0.52699   +0.88532   +1.87067
H   -0.55742   -0.85522   +1.89457
H   -1.01212   +0.07624   -0.38989
H   +0.56978   +0.84041   -0.39502
H   +0.42938   -0.91180   -0.41162

* E =  +9.485 kcal/mol ; Conformer 016
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51602
C   +1.38310   +0.00000   +2.14815
C   +2.23196   -1.19807   +1.75875
C   +3.03423   -0.97580   +0.50299
O   +3.63741   -2.03879   -0.04698
C   +3.50007   -3.32955   +0.49960
O   +3.19039   +0.09626   -0.00393
H   +4.17390   -3.96115   -0.06599
H   +3.78496   -3.35797   +1.54860
H   +2.48546   -3.70504   +0.38579
H   +2.95279   -1.42969   +2.54524
H   +1.61351   -2.08973   +1.65398
H   +1.91882   +0.90563   +1.87046
H   +1.27121   +0.01067   +3.23089
H   -0.53964   +0.87569   +1.87548
H   -0.55615   -0.86669   +1.87995
H   -1.01480   +0.06105   -0.38634
H   +0.57055   +0.83721   -0.39363
H   +0.44411   -0.90799   -0.40568

* E =  +9.744 kcal/mol ; Conformer 017
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51507
C   +1.39983   +0.00000   +2.09728
C   +1.39397   +0.01960   +3.62254
C   +2.79626   +0.08753   +4.16016
O   +3.45453   -1.05545   +4.39758
C   +2.82460   -2.30939   +4.27680
O   +3.36588   +1.12524   +4.33580
H   +3.60558   -3.04593   +4.42064
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H    +2.06511    -2.44601    +5.04347
H    +2.38324    -2.44978    +3.29311
H    +0.89317    +0.91845    +3.96961
H    +0.84680    -0.83777    +4.00758
H    +1.94410    -0.87326    +1.73305
H    +1.94849    +0.87167    +1.74201
H    -0.53870    +0.87407    +1.88279
H    -0.54496    -0.87082    +1.88294
H    -1.01199    +0.00259    -0.39711
H    +0.51176    +0.87724    -0.39101
H    +0.50753    -0.87925    -0.39292

* E =   +9.924 kcal/mol ; Conformer 018
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51578
C    +1.39166    +0.00000    +2.12779
C    +2.26856    -1.18310    +1.70956
C    +1.60681    -2.49583    +2.02153
O    +1.76926    -3.03216    +3.23850
C    +2.67936    -2.49154    +4.16830
O    +0.89279    -3.05594    +1.23975
H    +2.54284    -3.06205    +5.07874
H    +3.70615    -2.60910    +3.82904
H    +2.47797    -1.44354    +4.37394
H    +2.41534    -1.16877    +0.63433
H    +3.24607    -1.10138    +2.17737
H    +1.91467    +0.91126    +1.83683
H    +1.30515    +0.03073    +3.21409
H    -0.52589    +0.88055    +1.88396
H    -0.55931    -0.86414    +1.87309
H    -1.00790    +0.12806    -0.38665
H    +0.61093    +0.81141    -0.39527
H    +0.37965    -0.94039    -0.39140

* E =   +9.990 kcal/mol ; Conformer 019
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51507
C    +1.40525    +0.00000    +2.08629
C    +1.44870    -0.03974    +3.61441
C    +0.80833    +1.17971    +4.21676
O    +1.55014    +2.28552    +4.37414
C    +2.94478    +2.27604    +4.17475
O    -0.35093    +1.22178    +4.51262
H    +3.26503    +3.30424    +4.29027
H    +3.44554    +1.66485    +4.92246
H    +3.21333    +1.93149    +3.17959
H    +0.87339    -0.88931    +3.97010
H    +2.47298    -0.16210    +3.95683
```

```
H   +1.94723   -0.86943   +1.71371
H   +1.94379   +0.87424   +1.71623
H   -0.54968   +0.86301   +1.88712
H   -0.53437   -0.87496   +1.88618
H   -1.01276   -0.00529   -0.39481
H   +0.50175   +0.88275   -0.39329
H   +0.51401   -0.87455   -0.39594


* E = +10.264 kcal/mol ; Conformer 020
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51629
C   +1.38718   +0.00000   +2.13493
C   +2.18353   -1.26519   +1.82430
C   +3.48965   -1.25844   +2.56830
O   +4.56352   -0.70835   +1.98496
C   +4.53014   -0.25909   +0.65037
O   +3.59474   -1.67968   +3.68357
H   +5.48225   +0.22841   +0.48025
H   +4.43017   -1.09043   -0.04403
H   +3.73039   +0.45796   +0.48200
H   +1.63467   -2.13116   +2.18340
H   +2.32777   -1.37883   +0.75355
H   +1.93498   +0.88011   +1.79253
H   +1.30557   +0.08975   +3.21664
H   -0.53404   +0.87936   +1.87438
H   -0.55551   -0.86336   +1.88462
H   -1.01124   +0.07668   -0.39165
H   +0.56836   +0.84317   -0.39096
H   +0.43364   -0.91073   -0.40783


* E = +10.323 kcal/mol ; Conformer 021
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51620
C   +1.38871   +0.00000   +2.13187
C   +2.20719   -1.23740   +1.77024
C   +3.55102   -1.18925   +2.44153
O   +3.67984   -1.71324   +3.66864
C   +2.62971   -2.42298   +4.28276
O   +4.49837   -0.65325   +1.94416
H   +2.96941   -2.63918   +5.28824
H   +1.71724   -1.83416   +4.33687
H   +2.43179   -3.36056   +3.76792
H   +1.65340   -2.13954   +2.02177
H   +2.40641   -1.25225   +0.70396
H   +1.93930   +0.88165   +1.80485
H   +1.30049   +0.07940   +3.21585
H   -0.53262   +0.88002   +1.87512
H   -0.55828   -0.86301   +1.88322
```

```
H    -1.01094    +0.08807    -0.39003
H    +0.57980    +0.83490    -0.39009
H    +0.42439    -0.91506    -0.40714


* E = +11.690 kcal/mol ; Conformer 022
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51790
C    +1.39562    +0.00000    +2.13401
C    +1.97467    +1.39319    +2.39749
C    +1.92461    +2.29419    +1.19605
O    +2.90179    +2.21455    +0.28260
C    +4.06701    +1.45710    +0.51544
O    +1.01632    +3.04941    +0.99853
H    +4.63668    +1.50320    -0.40450
H    +4.66047    +1.88664    +1.31957
H    +3.84042    +0.41853    +0.73960
H    +1.37035    +1.88749    +3.15192
H    +2.98679    +1.30535    +2.78582
H    +1.37817    -0.51116    +3.09499
H    +2.06708    -0.57912    +1.49877
H    -0.55680    +0.86252    +1.88417
H    -0.53396    -0.88302    +1.86614
H    -1.01617    -0.00890    -0.38676
H    +0.49151    +0.87664    -0.41297
H    +0.50687    -0.88410    -0.38469


* E = +11.960 kcal/mol ; Conformer 023
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51524
C    +1.38974    +0.00000    +2.13029
C    +2.20708    -1.26068    +1.79946
C    +3.15203    -1.06578    +0.64660
O    +4.25401    -0.33026    +0.86203
C    +4.66894    +0.01122    +2.16478
O    +2.95967    -1.49836    -0.45235
H    +5.52596    +0.66152    +2.03935
H    +3.89903    +0.54263    +2.71762
H    +4.97539    -0.87204    +2.72142
H    +2.76834    -1.58593    +2.67274
H    +1.54518    -2.07490    +1.51980
H    +1.92309    +0.89117    +1.79571
H    +1.29780    +0.08631    +3.21173
H    -0.53718    +0.87445    +1.88226
H    -0.54687    -0.86930    +1.88400
H    -1.01526    +0.03309    -0.38790
H    +0.53205    +0.86648    -0.38994
H    +0.48522    -0.88444    -0.40480
```

S.2.2 $(\mathbf{TS}_{\alpha'})^{\ddagger}$

* E = +0.000 kcal/mol ; Conformer 001
```
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51490
C   +1.40214    +0.00000    +2.09420
C   +1.42355    -0.00454    +3.60808
C   +0.95491    +1.28635    +4.20039
O   +0.70913    +1.15706    +5.51628
C   +0.33269    +2.29902    +6.19637
O   +0.82126    +2.32435    +3.61732
H   +1.44868    +2.99575    +6.46431
H   -0.26498    +2.98295    +5.60758
H   -0.06095    +2.02383    +7.16404
H   +0.81861    -0.81075    +4.02045
H   +2.43316    -0.16577    +3.98779
H   +1.94308    -0.87576    +1.73593
H   +1.94197    +0.87550    +1.73544
H   -0.53557    +0.87572    +1.87966
H   -0.53977    -0.87505    +1.88170
H   -1.01165    -0.00585    -0.39836
H   +0.50333    +0.88329    -0.38857
H   +0.51619    -0.87422    -0.39385
H   +2.25195    +3.43301    +6.63079
```

* E = +0.001 kcal/mol ; Conformer 002
```
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51487
C   +1.40228    +0.00000    +2.09390
C   +1.42329    -0.00428    +3.60791
C   +0.95258    +1.28650    +4.19906
O   +0.71301    +1.16040    +5.51625
C   +0.29028    +2.29317    +6.18442
O   +0.82180    +2.32482    +3.61584
H   -1.02364    +2.43467    +5.94807
H   +0.36321    +2.12649    +7.24930
H   +0.72140    +3.21176    +5.80754
H   +0.81655    -0.80931    +4.01975
H   +2.43260    -0.16727    +3.98791
H   +1.94335    -0.87580    +1.73586
H   +1.94204    +0.87551    +1.73495
H   -0.53597    +0.87521    +1.87994
H   -0.53949    -0.87512    +1.88172
H   -1.01177    -0.00559    -0.39800
H   +0.50321    +0.88335    -0.38870
H   +0.51595    -0.87428    -0.39414
H   -1.93254    +2.48020    +5.75945
```

* E = +0.111 kcal/mol ; Conformer 003

```
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51508
C    +1.39984    +0.00000    +2.09718
C    +1.39515    -0.00006    +3.60906
C    +2.76902    -0.00559    +4.19512
O    +2.72310    +0.01381    +5.53985
C    +3.93278    -0.01441    +6.20591
O    +3.79858    -0.02024    +3.58365
H    +4.34855    -1.29035    +6.23525
H    +4.72955    +0.50619    +5.69029
H    +3.77541    +0.24868    +7.24186
H    +0.86889    +0.86813    +4.00688
H    +0.86692    -0.86774    +4.00555
H    +1.95168    -0.86891    +1.74040
H    +1.95145    +0.86887    +1.73961
H    -0.54488    +0.87197    +1.88066
H    -0.54443    -0.87223    +1.88058
H    -1.01144    -0.00024    -0.39892
H    +0.51084    +0.87801    -0.39103
H    +0.51122    -0.87782    -0.39088
H    +4.58541    -2.18955    +6.23471

*  E =   +0.671 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51677
C    +1.38930    +0.00000    +2.13452
C    +2.20565    -1.24024    +1.82913
C    +1.65285    -2.47142    +2.47329
O    +2.18336    -3.58430    +1.93553
C    +1.76872    -4.79099    +2.46479
O    +0.86315    -2.50379    +3.37377
H    +0.57719    -5.08197    +1.91963
H    +2.42832    -5.57530    +2.12296
H    +1.56585    -4.75789    +3.52755
H    +2.30244    -1.42436    +0.76164
H    +3.22504    -1.13083    +2.20184
H    +1.94297    +0.86961    +1.77995
H    +1.30097    +0.09705    +3.21477
H    -0.52989    +0.88273    +1.87280
H    -0.55755    -0.85741    +1.89181
H    -1.01230    +0.07317    -0.39003
H    +0.56693    +0.84293    -0.39341
H    +0.43427    -0.90964    -0.41021
H    -0.24016    -5.23771    +1.50521
21
*  E =   +0.680 kcal/mol ; Conformer 005
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51678
```

```
C    +1.38915    +0.00000    +2.13470
C    +2.20435    -1.24159    +1.83274
C    +1.65432    -2.47007    +2.48426
O    +2.18071    -3.58495    +1.94618
C    +1.80676    -4.78822    +2.51238
O    +0.86321    -2.49892    +3.38355
H    +2.54717    -4.96109    +3.61885
H    +0.78783    -4.80317    +2.87728
H    +2.09670    -5.59603    +1.85627
H    +2.30097    -1.42972    +0.76586
H    +3.22403    -1.13194    +2.20438
H    +1.94346    +0.86837    +1.77820
H    +1.30079    +0.09961    +3.21467
H    -0.53031    +0.88257    +1.87251
H    -0.55753    -0.85727    +1.89245
H    -1.01230    +0.07104    -0.39053
H    +0.56505    +0.84428    -0.39308
H    +0.43727    -0.90816    -0.41049
H    +3.09083    -5.03472    +4.36940

* E =  +0.688 kcal/mol ; Conformer 006
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51681
C    +1.38709    +0.00000    +2.13552
C    +2.18687    -1.24155    +1.80566
C    +3.50494    -1.28074    +2.50749
O    +4.20366    -2.37900    +2.16581
C    +5.43363    -2.54910    +2.77068
O    +3.92275    -0.46252    +3.27568
H    +5.21605    -3.06014    +3.99268
H    +5.98622    -3.31453    +2.24538
H    +5.95786    -1.62255    +2.96674
H    +1.64377    -2.14671    +2.08158
H    +2.38359    -1.33208    +0.73823
H    +1.93991    +0.87908    +1.80468
H    +1.30952    +0.08725    +3.21741
H    -0.53524    +0.87902    +1.87368
H    -0.55942    -0.86284    +1.88247
H    -1.01059    +0.08196    -0.39270
H    +0.57463    +0.83912    -0.38972
H    +0.43034    -0.91252    -0.40766
H    +5.01002    -3.42095    +4.82461

* E =  +0.690 kcal/mol ; Conformer 007
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51680
C    +1.38718    +0.00000    +2.13535
C    +2.18670    -1.24182    +1.80586
```

```
C    +3.50875    -1.27638    +2.50035
O    +4.19186    -2.39285    +2.18741
C    +5.44512    -2.53560    +2.75011
O    +3.93783    -0.44486    +3.24779
H    +6.30114    -1.80138    +2.02223
H    +5.52883    -2.11964    +3.74597
H    +5.77859    -3.55535    +2.62331
H    +1.64485    -2.14740    +2.08265
H    +2.38177    -1.33220    +0.73804
H    +1.94073    +0.87834    +1.80412
H    +1.30927    +0.08831    +3.21722
H    -0.53507    +0.87913    +1.87363
H    -0.55968    -0.86274    +1.88245
H    -1.01063    +0.08200    -0.39261
H    +0.57472    +0.83901    -0.38968
H    +0.43032    -0.91247    -0.40774
H    +6.85184    -1.28444    +1.47982


* E =   +0.741 kcal/mol ; Conformer 008
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51481
C    +1.40103    +0.00000    +2.09597
C    +1.41594    -0.03113    +3.61608
C    +0.71792    +1.13190    +4.24672
O    +1.09589    +2.29657    +3.68652
C    +0.49829    +3.44394    +4.16947
O    -0.06743    +1.07814    +5.14948
H    -0.70380    +3.53929    +3.58152
H    +0.27052    +3.40943    +5.22705
H    +1.04708    +4.30662    +3.82052
H    +0.93761    -0.92662    +4.00177
H    +2.44356    -0.02517    +3.97999
H    +1.94834    -0.86871    +1.73013
H    +1.94026    +0.88026    +1.74904
H    -0.54176    +0.87523    +1.87759
H    -0.54431    -0.87006    +1.88452
H    -1.01173    +0.00277    -0.39776
H    +0.51179    +0.87772    -0.39067
H    +0.50801    -0.87938    -0.39248
H    -1.51847    +3.54915    +3.13168


* E =   +0.832 kcal/mol ; Conformer 009
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51489
C    +1.40054    +0.00000    +2.09687
C    +1.41508    -0.02972    +3.61612
C    +0.74132    +1.14180    +4.25779
O    +1.08716    +2.29923    +3.66366
```

```
C    +0.56578    +3.45805    +4.20465
O    -0.00404    +1.09794    +5.19442
H    +1.31200    +3.77574    +5.27442
H    +0.71460    +4.27375    +3.51198
H    -0.43124    +3.34261    +4.60996
H    +0.92667    -0.91903    +4.00381
H    +2.44285    -0.03872    +3.97996
H    +1.94639    -0.87002    +1.73195
H    +1.94141    +0.87860    +1.74837
H    -0.54096    +0.87542    +1.87819
H    -0.54456    -0.87002    +1.88428
H    -1.01146    +0.00225    -0.39857
H    +0.51246    +0.87722    -0.39089
H    +0.50817    -0.87951    -0.39175
H    +1.86504    +3.95545    +5.99960

* E =   +0.960 kcal/mol ; Conformer 010
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51504
C    +1.40037    +0.00000    +2.09638
C    +1.39030    -0.00696    +3.61904
C    +2.76584    -0.01031    +4.19974
O    +3.43145    +1.11632    +3.88180
C    +4.73615    +1.21724    +4.32283
O    +3.25377    -0.88088    +4.86231
H    +5.50457    +0.52515    +3.46796
H    +5.06775    +2.24081    +4.22512
H    +4.91440    +0.73991    +5.27785
H    +0.86887    +0.87827    +3.98240
H    +0.87924    -0.88512    +4.00137
H    +1.94388    -0.87370    +1.73485
H    +1.94590    +0.87518    +1.74572
H    -0.54080    +0.87345    +1.88245
H    -0.54334    -0.87167    +1.88210
H    -1.01186    +0.00201    -0.39767
H    +0.51196    +0.87708    -0.39169
H    +0.50790    -0.87946    -0.39157
H    +5.98958    +0.04031    +2.83935

* E =   +0.979 kcal/mol ; Conformer 011
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51502
C    +1.40016    +0.00000    +2.09700
C    +1.38938    +0.00671    +3.61880
C    +2.75900    +0.01550    +4.21396
O    +3.46886    -1.05974    +3.82314
C    +4.75094    -1.17654    +4.32288
O    +3.20936    +0.85349    +4.94190
```

```
H    +4.65691    -1.67993    +5.56358
H    +5.28623    -1.92747    +3.76001
H    +5.25381    -0.22874    +4.46573
H    +0.87001    +0.87905    +4.00333
H    +0.87304    -0.88191    +3.98222
H    +1.94625    -0.87449    +1.74578
H    +1.94278    +0.87437    +1.73504
H    -0.54364    +0.87148    +1.88205
H    -0.54075    -0.87347    +1.88237
H    -1.01181    -0.00171    -0.39773
H    +0.50802    +0.87942    -0.39168
H    +0.51158    -0.87730    -0.39174
H    +4.53728    -2.03820    +6.41321

* E =  +1.016 kcal/mol ; Conformer 012
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51662
C    +1.38466    +0.00000    +2.14458
C    +2.24093    -1.18663    +1.73521
C    +2.92876    -0.98599    +0.42195
O    +3.13658    -2.15358    -0.21208
C    +3.78106    -2.08995    -1.43244
O    +3.29606    +0.06358    -0.02425
H    +2.86841    -1.70688    -2.34040
H    +4.54105    -1.32134    -1.48923
H    +4.07521    -3.08509    -1.73258
H    +3.03881    -1.34610    +2.46187
H    +1.66854    -2.11117    +1.69846
H    +1.91528    +0.91300    +1.87732
H    +1.28100    -0.00148    +3.22797
H    -0.53884    +0.87578    +1.87715
H    -0.55522    -0.86717    +1.87902
H    -1.01188    +0.09050    -0.38777
H    +0.59065    +0.82366    -0.39515
H    +0.41319    -0.92269    -0.40582
H    +2.18792    -1.44537    -2.91639

* E =  +1.057 kcal/mol ; Conformer 013
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51641
C    +1.39013    +0.00000    +2.13159
C    +2.25566    -1.17845    +1.69461
C    +1.57081    -2.48486    +1.92852
O    +1.32209    -2.67850    +3.23753
C    +0.62606    -3.82180    +3.57713
O    +1.25002    -3.27693    +1.08844
H    -0.67142    -3.57822    +3.33740
H    +0.85084    -4.67564    +2.95099
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H    +0.68922   -3.97482   +4.64467
H    +2.49198   -1.12937   +0.63696
H    +3.19020   -1.17380   +2.25279
H    +1.91188   +0.91765   +1.86006
H    +1.30670   -0.00806   +3.21664
H    -0.53692   +0.87365   +1.88420
H    -0.55609   -0.86680   +1.87906
H    -1.01007   +0.10039   -0.38914
H    +0.58963   +0.82770   -0.39280
H    +0.40931   -0.92548   -0.39930
H    -1.55223   -3.33944   +3.15509

* E =  +1.125 kcal/mol ; Conformer 014
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.51640
C    +1.38529   +0.00000   +2.14286
C    +2.24007   +1.18755   +1.73627
C    +2.95926   +0.98493   +0.44013
O    +3.24959   +2.15912   -0.14808
C    +3.99109   +2.10656   -1.31261
O    +3.28159   -0.06897   -0.02951
H    +5.27826   +1.94811   -0.96423
H    +3.78047   +1.24112   -1.92761
H    +3.95307   +3.06861   -1.80261
H    +1.66337   +2.10891   +1.68014
H    +3.02320   +1.36486   +2.47482
H    +1.28152   -0.00124   +3.22619
H    +1.91564   -0.91246   +1.87344
H    -0.55479   +0.86747   +1.87875
H    -0.53928   -0.87556   +1.87661
H    -1.01227   -0.08265   -0.38853
H    +0.42128   +0.92050   -0.40276
H    +0.58571   -0.82769   -0.39385
H    +6.15343   +1.84731   -0.66820

* E =  +1.210 kcal/mol ; Conformer 015
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.51648
C    +1.38945   +0.00000   +2.13276
C    +2.25398   -1.17851   +1.69772
C    +1.58461   -2.49164   +1.94176
O    +1.29448   -2.65709   +3.24583
C    +0.67848   -3.84014   +3.60379
O    +1.30678   -3.30977   +1.11146
H    +1.63064   -4.78224   +3.68804
H    +0.28922   -3.75038   +4.60761
H    -0.00049   -4.22540   +2.85390
H    +2.48750   -1.13480   +0.63922
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H   +3.19177   -1.16897   +2.25074
H   +1.91088   +0.91755   +1.86027
H   +1.30529   -0.00594   +3.21775
H   -0.53826   +0.87305   +1.88374
H   -0.55505   -0.86737   +1.87939
H   -1.00995   +0.09960   -0.38975
H   +0.58866   +0.82857   -0.39209
H   +0.41136   -0.92411   -0.40038
H   +2.32898   -5.39377   +3.74077


* E =  +1.512 kcal/mol ; Conformer 016
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51631
C   +1.38811   +0.00000   +2.13376
C   +2.18964   -1.25145   +1.79520
C   +3.51391   -1.27552   +2.48337
O   +4.29403   -0.25701   +2.07367
C   +5.53396   -0.14030   +2.67011
O   +3.87420   -2.07331   +3.30119
H   +5.35689   +0.47362   +3.84990
H   +5.98416   -1.08831   +2.93519
H   +6.14445   +0.53997   +2.09413
H   +1.65556   -2.14793   +2.09615
H   +2.36822   -1.30112   +0.72232
H   +1.94144   +0.87681   +1.79920
H   +1.29852   +0.07956   +3.21672
H   -0.53247   +0.88039   +1.87447
H   -0.55855   -0.86201   +1.88384
H   -1.01086   +0.08651   -0.39079
H   +0.57835   +0.83602   -0.39066
H   +0.42459   -0.91500   -0.40765
H   +5.17727   +0.91041   +4.65146


* E =  +1.532 kcal/mol ; Conformer 017
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51633
C   +1.38847   +0.00000   +2.13317
C   +2.18964   -1.25036   +1.79340
C   +3.51615   -1.28849   +2.47711
O   +4.26861   -0.22308   +2.14277
C   +5.53091   -0.15142   +2.69814
O   +3.89787   -2.13230   +3.23697
H   +6.33455   -0.95136   +1.98011
H   +5.92899   +0.84233   +2.55234
H   +5.59246   -0.55523   +3.70052
H   +1.65424   -2.14890   +2.08586
H   +2.37163   -1.29696   +0.72063
H   +1.94104   +0.87754   +1.79952
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H    +1.29829    +0.07892    +3.21634
H    -0.53284    +0.88016    +1.87454
H    -0.55819    -0.86232    +1.88369
H    -1.01088    +0.08635    -0.39075
H    +0.57823    +0.83605    -0.39075
H    +0.42475    -0.91492    -0.40756
H    +6.84957    -1.51096    +1.44501

* E =   +1.539 kcal/mol ; Conformer 018
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51634
C    +1.38704    +0.00000    +2.13594
C    +2.19349    -1.24731    +1.79181
C    +3.51932    -1.26175    +2.47823
O    +3.37621    -1.37951    +3.81226
C    +4.53052    -1.35410    +4.56958
O    +4.59164    -1.17422    +1.95142
H    +4.88003    -0.06854    +4.72744
H    +4.31057    -1.70442    +5.56765
H    +5.38681    -1.79834    +4.07856
H    +1.63743    -2.13289    +2.09907
H    +2.38881    -1.31368    +0.72705
H    +1.93467    +0.88207    +1.80163
H    +1.30185    +0.07293    +3.21850
H    -0.53386    +0.87951    +1.87463
H    -0.55687    -0.86334    +1.88410
H    -1.01108    +0.08314    -0.39096
H    +0.57551    +0.83803    -0.39033
H    +0.42917    -0.91280    -0.40736
H    +5.06961    +0.83841    +4.81329

* E =   +1.598 kcal/mol ; Conformer 019
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51681
C    +1.38153    +0.00000    +2.15100
C    +2.20163    -1.25478    +1.88590
C    +2.75378    -1.39979    +0.50342
O    +3.27306    -0.24501    +0.04816
C    +3.82154    -0.26754    -1.21900
O    +2.78771    -2.41403    -0.13412
H    +2.80961    -0.19454    -2.10139
H    +4.39215    +0.63621    -1.37651
H    +4.31199    -1.19956    -1.46895
H    +3.06556    -1.26735    +2.55193
H    +1.62988    -2.15604    +2.08990
H    +1.94323    +0.87076    +1.81549
H    +1.27074    +0.09785    +3.22985
H    -0.53394    +0.88077    +1.87283
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H   -0.56124    -0.86147    +1.88248
H   -1.01010    +0.11217    -0.38684
H   +0.59955    +0.81949    -0.39254
H   +0.39512    -0.92584    -0.41275
H   +2.08224    -0.13604    -2.67673


* E =   +1.829 kcal/mol ; Conformer 020
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51698
C   +1.38172    +0.00000    +2.15037
C   +2.20925    -1.24554    +1.86581
C   +2.77616    -1.35892    +0.48627
O   +3.28519    -0.18994    +0.05733
C   +3.88402    -0.19104    -1.18688
O   +2.82107    -2.35922    -0.17229
H   +5.12231    -0.68926    -1.04079
H   +3.41782    -0.86203    -1.89687
H   +4.03345    +0.82853    -1.51170
H   +3.06817    -1.26849    +2.53785
H   +1.64055    -2.15381    +2.04614
H   +1.93802    +0.87897    +1.82754
H   +1.27013    +0.08228    +3.23038
H   -0.53510    +0.87980    +1.87346
H   -0.56036    -0.86262    +1.88099
H   -1.00996    +0.11301    -0.38683
H   +0.60045    +0.81987    -0.39076
H   +0.39414    -0.92803    -0.40889
H   +5.97258    -1.03057    -0.88553


* E =   +6.868 kcal/mol ; Conformer 021
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51481
C   +1.40316    +0.00000    +2.09148
C   +1.42378    -0.00007    +3.60657
C   +0.98168    +1.31632    +4.18103
O   +0.76076    +1.37569    +5.51371
C   +0.92677    +0.28079    +6.32768
O   +0.83446    +2.31409    +3.54303
H   -0.06221    -0.58661    +6.11448
H   +1.83385    -0.29023    +6.15723
H   +0.78361    +0.58463    +7.35527
H   +0.79737    -0.79913    +4.00237
H   +2.43227    -0.19236    +3.97857
H   +1.94055    -0.88025    +1.73865
H   +1.94473    +0.87273    +1.73031
H   -0.53450    +0.87540    +1.88023
H   -0.53855    -0.87572    +1.88178
H   -1.01204    -0.00784    -0.39709
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H   +0.50049   +0.88491   -0.38840
H   +0.51766   -0.87294   -0.39495
H   -0.77680   -1.17473   +5.93101


* E =  +6.987 kcal/mol ; Conformer 022
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51515
C   +1.40072   +0.00000   +2.09478
C   +1.39807   -0.00283   +3.60768
C   +2.78752   +0.01153   +4.17434
O   +2.91845   -0.10170   +5.51615
C   +1.82973   -0.24364   +6.34254
O   +3.77882   +0.12329   +3.52003
H   +1.31121   -1.46182   +6.19043
H   +2.16701   -0.23495   +7.36964
H   +1.00377   +0.43143   +6.14266
H   +0.86426   +0.87114   +3.98792
H   +0.86387   -0.87047   +3.99597
H   +1.95255   -0.86897   +1.73861
H   +1.95474   +0.86786   +1.74086
H   -0.54426   +0.87290   +1.87999
H   -0.54514   -0.87189   +1.88049
H   -1.01148   +0.00046   -0.39864
H   +0.51163   +0.87749   -0.39089
H   +0.51041   -0.87828   -0.39068
H   +0.97301   -2.33193   +6.05197


* E =  +7.074 kcal/mol ; Conformer 023
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51478
C   +1.40311   +0.00000   +2.09177
C   +1.43016   +0.00292   +3.60691
C   +1.04359   +1.33451   +4.18480
O   +1.01592   +1.44676   +5.53262
C   +1.34185   +0.39971   +6.36103
O   +0.77279   +2.29962   +3.53728
H   +2.65153   +0.15784   +6.28196
H   +1.20086   +0.71002   +7.38698
H   +0.87418   -0.54903   +6.11868
H   +0.75691   -0.76228   +3.99739
H   +2.42051   -0.24874   +3.98717
H   +1.93869   -0.88155   +1.73939
H   +1.94621   +0.87042   +1.72674
H   -0.53524   +0.87394   +1.88129
H   -0.53665   -0.87788   +1.88048
H   -1.01197   -0.01039   -0.39725
H   +0.49791   +0.88649   -0.38810
H   +0.52029   -0.87124   -0.39534
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H    +3.58002    +0.01778    +6.20108

* E =  +7.420 kcal/mol ; Conformer 024
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51697
C    +1.38902    +0.00000    +2.13540
C    +2.21476    -1.22745    +1.80080
C    +1.67300    -2.47076    +2.44736
O    +2.16729    -3.66001    +2.03360
C    +3.12647    -3.74575    +1.05348
O    +0.85465    -2.47584    +3.31601
H    +2.57884    -3.45190    -0.12487
H    +3.95418    -3.05073    +1.15297
H    +3.42735    -4.77874    +0.94779
H    +2.28854    -1.37228    +0.72503
H    +3.23983    -1.10253    +2.15651
H    +1.93635    +0.87880    +1.79364
H    +1.30180    +0.07517    +3.21694
H    -0.52718    +0.88410    +1.87346
H    -0.55770    -0.85626    +1.89274
H    -1.01162    +0.08763    -0.38864
H    +0.57819    +0.83479    -0.39483
H    +0.41922    -0.91630    -0.41198
H    +2.14552    -3.22858    -0.93361

* E =  +7.538 kcal/mol ; Conformer 025
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51692
C    +1.38624    +0.00000    +2.13714
C    +2.18467    -1.24443    +1.81067
C    +3.51177    -1.25732    +2.51126
O    +4.36425    -2.26651    +2.21823
C    +4.04657    -3.24377    +1.30605
O    +3.85960    -0.44242    +3.31017
H    +4.07006    -2.73068    +0.07630
H    +4.83858    -3.97952    +1.29194
H    +3.05201    -3.66663    +1.40598
H    +1.63062    -2.13789    +2.10912
H    +2.35504    -1.34169    +0.73918
H    +1.94341    +0.87447    +1.80245
H    +1.31208    +0.09103    +3.21836
H    -0.53349    +0.88019    +1.87325
H    -0.56212    -0.86096    +1.88350
H    -1.01040    +0.08492    -0.39244
H    +0.57699    +0.83738    -0.38958
H    +0.42770    -0.91313    -0.40936
H    +4.09383    -2.32905    -0.77752
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* E =  +7.554 kcal/mol ; Conformer 026
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51687
C   +1.38638   +0.00000   +2.13671
C   +2.18378   -1.24607   +1.81322
C   +3.51895   -1.24678   +2.49793
O   +4.28025   -2.35976   +2.38568
C   +3.85538   -3.46283   +1.68518
O   +3.95343   -0.32994   +3.12564
H   +2.88519   -4.07494   +2.36341
H   +3.41986   -3.25604   +0.71282
H   +4.65307   -4.19226   +1.66429
H   +1.63541   -2.14456   +2.09937
H   +2.35739   -1.32966   +0.73901
H   +1.94524   +0.87387   +1.80491
H   +1.30908   +0.09057   +3.21821
H   -0.53270   +0.88091   +1.87259
H   -0.56260   -0.86044   +1.88320
H   -1.01006   +0.08819   -0.39253
H   +0.57988   +0.83527   -0.39002
H   +0.42319   -0.91562   -0.40888
H   +2.20006   -4.47728   +2.87268

* E =  +7.801 kcal/mol ; Conformer 027
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51684
C   +1.38952   +0.00000   +2.13461
C   +2.20420   -1.24774   +1.85120
C   +1.69697   -2.44709   +2.59907
O   +2.34330   -3.62082   +2.41044
C   +3.44149   -3.72836   +1.59145
O   +0.77352   -2.43288   +3.35488
H   +4.47793   -3.10128   +2.15016
H   +3.75422   -4.76281   +1.56162
H   +3.34030   -3.26959   +0.61325
H   +2.21373   -1.47169   +0.78433
H   +3.24847   -1.10181   +2.12886
H   +1.94738   +0.85953   +1.76213
H   +1.30376   +0.11742   +3.21272
H   -0.52467   +0.88697   +1.86989
H   -0.55938   -0.85350   +1.89474
H   -1.01237   +0.07622   -0.38914
H   +0.56925   +0.84061   -0.39513
H   +0.42861   -0.91166   -0.41278
H   +5.18669   -2.65007   +2.57751

* E =  +8.173 kcal/mol ; Conformer 028
C   +0.00000   +0.00000   +0.00000
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C    +0.00000    +0.00000    +1.51614
C    +1.38393    +0.00000    +2.14668
C    +2.23513    +1.18906    +1.73360
C    +3.01563    +0.94057    +0.47236
O    +3.56492    +2.01099    -0.14589
C    +3.41739    +3.28811    +0.33937
O    +3.21255    -0.13791    +0.00148
H    +2.16588    +3.69320    +0.13141
H    +3.57094    +3.39870    +1.40813
H    +4.01043    +3.96144    -0.26376
H    +1.62105    +2.08208    +1.62431
H    +2.97173    +1.42096    +2.50599
H    +1.27585    +0.00881    +3.22961
H    +1.91427    -0.91324    +1.88400
H    -0.55465    +0.86795    +1.87841
H    -0.53965    -0.87490    +1.87730
H    -1.01436    -0.06777    -0.38592
H    +0.43423    +0.91357    -0.40479
H    +0.57460    -0.83413    -0.39508
H    +1.26604    +3.92538    -0.03540

* E =   +8.513 kcal/mol ; Conformer 029
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51501
C    +1.40027    +0.00000    +2.09633
C    +1.39208    -0.01651    +3.62209
C    +2.78894    -0.08505    +4.16581
O    +3.44257    +1.07146    +4.42012
C    +2.85188    +2.29962    +4.24359
O    +3.37277    -1.11035    +4.34726
H    +1.92763    +2.48497    +5.18482
H    +3.58313    +3.07073    +4.44246
H    +2.31852    +2.42702    +3.30694
H    +0.84666    +0.83919    +4.01228
H    +0.89207    -0.91582    +3.96912
H    +1.94822    -0.87250    +1.74208
H    +1.94466    +0.87209    +1.72901
H    -0.54462    +0.87060    +1.88339
H    -0.53827    -0.87410    +1.88306
H    -1.01217    -0.00298    -0.39644
H    +0.50668    +0.87962    -0.39314
H    +0.51179    -0.87705    -0.39138
H    +1.27641    +2.56872    +5.86211

* E =   +8.579 kcal/mol ; Conformer 030
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51583
C    +1.38298    +0.00000    +2.14841
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C    +2.22946    +1.20441    +1.76992
C    +3.07996    +0.97290    +0.55297
O    +3.82436    +2.01178    +0.10752
C    +3.83085    +3.23463    +0.73442
O    +3.16222    -0.06304    -0.03284
H    +4.44311    +3.13045    +1.91567
H    +4.46688    +3.90797    +0.17681
H    +2.85373    +3.64434    +0.96871
H    +1.59456    +2.07636    +1.60279
H    +2.90432    +1.48401    +2.57940
H    +1.27116    -0.01743    +3.23080
H    +1.91932    -0.90410    +1.86669
H    -0.55507    +0.86726    +1.88005
H    -0.54049    -0.87491    +1.87570
H    -1.01558    -0.04579    -0.38625
H    +0.45898    +0.90062    -0.40538
H    +0.55763    -0.84573    -0.39375
H    +4.88492    +3.02149    +2.74087

* E =   +8.718 kcal/mol ; Conformer 031
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51581
C    +1.39155    +0.00000    +2.12813
C    +2.26989    +1.18193    +1.70867
C    +1.61395    +2.49558    +2.01579
O    +1.79918    +3.04536    +3.23715
C    +2.64228    +2.48973    +4.16987
O    +0.89483    +3.06468    +1.24996
H    +3.90317    +2.64002    +3.76647
H    +2.58859    +3.07156    +5.07949
H    +2.52906    +1.42129    +4.32039
H    +3.24944    +1.10696    +2.17260
H    +2.41365    +1.16665    +0.63306
H    +1.30448    -0.03243    +3.21443
H    +1.91534    -0.91047    +1.83694
H    -0.56066    +0.86321    +1.87365
H    -0.52555    -0.88076    +1.88363
H    -1.00788    -0.12829    -0.38642
H    +0.37949    +0.93977    -0.39307
H    +0.61088    -0.81143    -0.39503
H    +4.77755    +2.75905    +3.43427

* E =   +8.737 kcal/mol ; Conformer 032
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51503
C    +1.40501    +0.00000    +2.08680
C    +1.44762    -0.03945    +3.61528
C    +0.81400    +1.17897    +4.22005
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O   +1.57720   +2.28227   +4.39723
C   +2.92924   +2.28726   +4.14992
O   -0.34116   +1.24615   +4.51517
H   +3.54541   +1.54727   +5.06997
H   +3.23129   +1.85185   +3.20319
H   +3.31121   +3.28452   +4.31857
H   +0.86553   -0.88491   +3.96975
H   +2.46808   -0.16647   +3.96624
H   +1.94673   -0.87054   +1.71710
H   +1.94454   +0.87269   +1.71420
H   -0.55034   +0.86315   +1.88619
H   -0.53418   -0.87514   +1.88594
H   -1.01282   -0.00583   -0.39447
H   +0.50128   +0.88288   -0.39349
H   +0.51425   -0.87440   -0.39568
H   +3.93491   +1.00359   +5.73539


* E =  +8.842 kcal/mol ; Conformer 033
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51512
C   +1.40065   +0.00000   +2.09367
C   +1.39372   +0.01312   +3.61904
C   +2.79988   +0.09424   +4.13841
O   +3.37422   -1.00638   +4.67569
C   +2.66847   -2.15098   +4.95730
O   +3.46350   +1.08252   +4.04878
H   +2.21564   -2.70853   +3.83040
H   +3.35060   -2.89100   +5.35252
H   +1.77931   -2.00394   +5.56292
H   +0.88590   +0.90893   +3.96874
H   +0.85002   -0.84858   +3.99316
H   +1.94011   -0.87914   +1.73914
H   +1.95250   +0.87094   +1.74290
H   -0.54053   +0.87335   +1.88288
H   -0.54211   -0.87296   +1.88174
H   -1.01206   +0.00049   -0.39705
H   +0.51041   +0.87794   -0.39128
H   +0.50920   -0.87878   -0.39130
H   +1.89914   -3.08459   +3.02858


* E =  +9.010 kcal/mol ; Conformer 034
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51626
C   +1.38762   +0.00000   +2.13397
C   +2.17804   +1.27036   +1.82696
C   +3.49254   +1.26267   +2.54995
O   +4.56951   +0.73032   +1.92833
C   +4.50822   +0.24971   +0.64228
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O    +3.63099    +1.66422    +3.66564
H    +4.37973    +1.26968    -0.20461
H    +5.46504    -0.18303    +0.38512
H    +3.65983    -0.39207    +0.42681
H    +2.31217    +1.40269    +0.75737
H    +1.63286    +2.13057    +2.20491
H    +1.30814    -0.09604    +3.21527
H    +1.93626    -0.87769    +1.78632
H    -0.55536    +0.86316    +1.88519
H    -0.53327    -0.87954    +1.87488
H    -1.01168    -0.07314    -0.39100
H    +0.43698    +0.90854    -0.40888
H    +0.56447    -0.84576    -0.39100
H    +4.27649    +2.02101    -0.76583

* E =  +9.091 kcal/mol ; Conformer 035
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51615
C    +1.38885    +0.00000    +2.13168
C    +2.20600    +1.23737    +1.76497
C    +3.54957    +1.19746    +2.43084
O    +3.67947    +1.74850    +3.65960
C    +2.63951    +2.39089    +4.28734
O    +4.50459    +0.66464    +1.95221
H    +2.39534    +3.54527    +3.66929
H    +1.69036    +1.86476    +4.26894
H    +2.95897    +2.68852    +5.27643
H    +2.40548    +1.24632    +0.69865
H    +1.65811    +2.14419    +2.01101
H    +1.30015    -0.07806    +3.21587
H    +1.93853    -0.88285    +1.80646
H    -0.55817    +0.86285    +1.88321
H    -0.53174    -0.88032    +1.87546
H    -1.01098    -0.08989    -0.38927
H    +0.42176    +0.91613    -0.40738
H    +0.58086    -0.83398    -0.39054
H    +2.25031    +4.34763    +3.19469

* E =  +9.215 kcal/mol ; Conformer 036
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51618
C    +1.39125    +0.00000    +2.12758
C    +2.24826    -1.19939    +1.72075
C    +1.54394    -2.51788    +1.86911
O    +1.38131    -3.04732    +3.10195
C    +1.73534    -2.40443    +4.26180
O    +1.11201    -3.13547    +0.94185
H    +0.71865    -1.64685    +4.65398
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H    +1.82465    -3.13217    +5.05697
H    +2.57840    -1.72658    +4.18665
H    +2.49961    -1.13683    +0.66723
H    +3.18494    -1.19943    +2.27600
H    +1.92525    +0.89821    +1.81727
H    +1.30658    +0.05461    +3.21067
H    -0.53129    +0.87653    +1.88508
H    -0.55836    -0.86423    +1.88042
H    -1.01091    +0.09696    -0.38759
H    +0.58480    +0.83210    -0.39106
H    +0.41233    -0.92425    -0.39746
H    -0.02851    -1.12249    +4.90281

* E =   +9.227 kcal/mol ; Conformer 037
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51429
C    +1.40491    +0.00000    +2.08565
C    +1.44510    +0.07602    +3.61120
C    +0.45913    -0.82507    +4.30132
O    +0.66077    -2.16220    +4.28693
C    +1.69305    -2.76847    +3.61607
O    -0.50645    -0.41909    +4.87467
H    +1.31651    -2.99133    +2.36275
H    +2.60712    -2.18966    +3.53899
H    +1.83503    -3.76496    +4.01207
H    +2.45302    -0.11851    +3.97673
H    +1.17031    +1.07382    +3.93706
H    +1.93415    -0.88082    +1.72654
H    +1.95638    +0.85771    +1.70101
H    -0.54771    +0.86352    +1.89241
H    -0.53786    -0.87867    +1.87489
H    -1.01215    -0.00788    -0.39598
H    +0.50412    +0.88075    -0.39430
H    +0.51407    -0.87789    -0.38832
H    +1.01407    -3.14091    +1.47751

* E =   +9.266 kcal/mol ; Conformer 038
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51498
C    +1.40109    +0.00000    +2.09566
C    +1.38651    -0.02474    +3.61988
C    +2.76056    -0.12941    +4.21373
O    +3.52541    +0.98236    +4.30430
C    +3.17383    +2.20274    +3.78415
O    +3.22390    -1.15439    +4.61463
H    +3.60127    +2.28009    +2.53028
H    +2.11000    +2.40292    +3.72396
H    +3.73916    +2.97762    +4.28419
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H    +0.85584    +0.84387    +4.00746
H    +0.85808    -0.90794    +3.96487
H    +1.94572    -0.87304    +1.73640
H    +1.94368    +0.87124    +1.73025
H    -0.54305    +0.87218    +1.88264
H    -0.54049    -0.87280    +1.88299
H    -1.01217    +0.00143    -0.39655
H    +0.51131    +0.87692    -0.39275
H    +0.50778    -0.87955    -0.39101
H    +3.91822    +2.31565    +1.63914


* E =  +9.339 kcal/mol ; Conformer 039
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51566
C    +1.39000    +0.00000    +2.12971
C    +2.28625    +1.16802    +1.70348
C    +1.65332    +2.48323    +2.04436
O    +1.95969    +3.07152    +3.22484
C    +3.07330    +2.73115    +3.95409
O    +0.82994    +3.00924    +1.35709
H    +2.97407    +1.50067    +4.46977
H    +3.99848    +2.70478    +3.38601
H    +3.11833    +3.36091    +4.83195
H    +3.26518    +1.05094    +2.15770
H    +2.41391    +1.15985    +0.62511
H    +1.31124    -0.01388    +3.21574
H    +1.90950    -0.91605    +1.84793
H    -0.56318    +0.86071    +1.87356
H    -0.52188    -0.88318    +1.88325
H    -1.00695    -0.13256    -0.38762
H    +0.37467    +0.94257    -0.39165
H    +0.61526    -0.80765    -0.39633
H    +2.92997    +0.64205    +4.84913


* E =  +9.396 kcal/mol ; Conformer 040
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51533
C    +1.40643    +0.00000    +2.08223
C    +1.46376    +0.03989    +3.61174
C    +0.89169    -1.21528    +4.19954
O    +1.72706    -2.25418    +4.44379
C    +3.08704    -2.09825    +4.56160
O    -0.27450    -1.38137    +4.39396
H    +3.66061    -1.77384    +3.39731
H    +3.39641    -1.30403    +5.23477
H    +3.52732    -3.05907    +4.79040
H    +2.48674    +0.20911    +3.93342
H    +0.85218    +0.85987    +3.97781
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H   +1.95199   -0.87082   +1.71783
H   +1.94643   +0.87138   +1.71177
H   -0.53389   +0.87606   +1.88545
H   -0.54935   -0.86309   +1.88662
H   -1.01285   +0.00617   -0.39468
H   +0.51512   +0.87378   -0.39612
H   +0.50123   -0.88321   -0.39241
H   +4.09903   -1.54827   +2.59674


* E =  +9.879 kcal/mol ; Conformer 041
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51619
C   +1.38740   +0.00000   +2.13610
C   +2.20045   -1.23875   +1.77162
C   +3.56166   -1.23249   +2.40240
O   +3.69069   -1.61275   +3.69425
C   +2.63504   -1.90544   +4.52086
O   +4.55141   -0.90305   +1.82118
H   +2.23688   -0.79485   +5.12789
H   +1.74373   -2.28551   +4.03468
H   +2.98499   -2.51990   +5.33948
H   +1.64911   -2.14181   +2.03140
H   +2.38490   -1.26513   +0.70335
H   +1.93627   +0.88200   +1.80601
H   +1.29443   +0.08312   +3.21741
H   -0.53187   +0.88026   +1.87503
H   -0.55948   -0.86206   +1.88375
H   -1.01095   +0.09043   -0.38935
H   +0.58090   +0.83409   -0.39029
H   +0.42156   -0.91567   -0.40870
H   +1.97086   +0.00830   +5.55295


* E = +10.499 kcal/mol ; Conformer 042
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51790
C   +1.39543   +0.00000   +2.13401
C   +1.97576   -1.39306   +2.39723
C   +1.92290   -2.29918   +1.20301
O   +2.91699   -2.23035   +0.28902
C   +4.03128   -1.44811   +0.48052
O   +1.02378   -3.05787   +0.99521
H   +4.77588   -1.97973   +1.44909
H   +4.65913   -1.51318   -0.39713
H   +3.83604   -0.43394   +0.81139
H   +2.98961   -1.31237   +2.78181
H   +1.37199   -1.88606   +3.15290
H   +2.06558   +0.58234   +1.50022
H   +1.37810   +0.50848   +3.09616
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H    -0.53349    +0.88335    +1.86560
H    -0.55787    -0.86153    +1.88506
H    -1.01598    +0.01015    -0.38696
H    +0.50806    +0.88321    -0.38487
H    +0.48960    -0.87728    -0.41423
H    +5.26181    -2.38677    +2.14726


* E = +10.693 kcal/mol ; Conformer 043
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51522
C    +1.38959    +0.00000    +2.13053
C    +2.20735    +1.26088    +1.79969
C    +3.15222    +1.06757    +0.65035
O    +4.27383    +0.34340    +0.87923
C    +4.65582    -0.03490    +2.14458
O    +2.97309    +1.48333    -0.45411
H    +5.04226    +1.04336    +2.82239
H    +3.87682    -0.47408    +2.75872
H    +5.55238    -0.63494    +2.07363
H    +1.54542    +2.07350    +1.51584
H    +2.77044    +1.59097    +2.66967
H    +1.29814    -0.08386    +3.21211
H    +1.92132    -0.89301    +1.79786
H    -0.54708    +0.86893    +1.88425
H    -0.53667    -0.87466    +1.88209
H    -1.01507    -0.03662    -0.38776
H    +0.48077    +0.88662    -0.40544
H    +0.53476    -0.86459    -0.39054
H    +5.29439    +1.83790    +3.26690


* E = +10.749 kcal/mol ; Conformer 044
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51787
C    +1.39103    +0.00000    +2.14253
C    +1.98914    +1.39331    +2.34159
C    +2.03871    +2.23663    +1.10222
O    +2.99376    +1.99487    +0.17573
C    +3.91450    +0.98077    +0.26879
O    +1.26764    +3.12248    +0.88265
H    +3.42978    -0.11700    -0.30290
H    +4.76700    +1.21877    -0.35312
H    +4.17577    +0.67144    +1.27439
H    +1.36511    +1.95306    +3.03118
H    +2.97857    +1.31616    +2.78919
H    +1.35012    -0.45680    +3.12989
H    +2.05629    -0.62521    +1.54748
H    -0.56069    +0.85924    +1.88766
H    -0.53411    -0.88380    +1.86393
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H   -1.01709   -0.00247   -0.38462
H   +0.49584   +0.87197   -0.41866
H   +0.50242   -0.88534   -0.38525
H   +3.09632   -0.89610   -0.71919


* E = +11.361 kcal/mol ; Conformer 045
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51787
C   +1.39708   +0.00000   +2.13155
C   +1.95492   +1.38960   +2.46005
C   +1.91962   +2.31103   +1.27930
O   +2.96433   +2.30104   +0.41634
C   +4.21484   +1.86358   +0.78132
O   +0.98300   +3.00275   +1.01430
H   +4.26730   +0.53828   +0.96514
H   +4.89063   +2.01470   -0.04921
H   +4.57943   +2.26902   +1.72063
H   +1.32996   +1.85490   +3.21658
H   +2.95841   +1.28777   +2.86448
H   +1.39461   -0.55242   +3.06941
H   +2.08629   -0.52642   +1.47232
H   -0.56011   +0.86032   +1.88433
H   -0.53235   -0.88425   +1.86531
H   -1.01575   +0.00059   -0.38812
H   +0.50108   +0.87218   -0.41097
H   +0.50082   -0.88733   -0.38418
H   +4.36547   -0.38627   +1.09644


* E = +11.626 kcal/mol ; Conformer 046
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51525
C   +1.38249   +0.00000   +2.14535
C   +2.21128   +1.25949   +1.83823
C   +3.11159   +1.08147   +0.65261
O   +4.22381   +0.32222   +0.82907
C   +4.83325   +0.19227   +2.05370
O   +2.89250   +1.50182   -0.44201
H   +4.12452   -0.51980   +2.93850
H   +5.72613   -0.40608   +1.93394
H   +5.00599   +1.13164   +2.57171
H   +1.55849   +2.09801   +1.61338
H   +2.80416   +1.52910   +2.70899
H   +1.27871   -0.08399   +3.22502
H   +1.92994   -0.88825   +1.82897
H   -0.55369   +0.86581   +1.88246
H   -0.53502   -0.87678   +1.87980
H   -1.01446   -0.06481   -0.38611
H   +0.45490   +0.89945   -0.40587
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H    +0.55772    -0.84970    -0.39112
H    +3.70033    -1.01358    +3.61810
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S.2.3 $(\text{TS}_\alpha)^\ddagger$

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* E =  +0.000 kcal/mol ; Conformer 001
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51512
C    +1.40825    +0.00000    +2.09114
C    +1.41455    +0.01214    +3.59001
C    +1.00953    -1.25087    +4.24186
O    +0.73444    -1.07965    +5.53362
C    +0.39234    -2.25826    +6.24036
O    +0.96198    -2.32335    +3.69607
H    +1.20719    -2.97438    +6.19964
H    +0.20735    -1.94864    +7.26067
H    -0.49554    -2.71264    +5.81182
H    +2.63385    +0.14822    +3.95157
H    +0.96387    +0.88154    +4.05779
H    +1.93774    -0.88585    +1.74399
H    +1.95282    +0.87026    +1.72503
H    -0.54129    +0.87254    +1.88362
H    -0.52925    -0.87836    +1.88259
H    -1.01265    -0.00066    -0.39584
H    +0.50965    +0.87780    -0.39391
H    +0.50840    -0.88008    -0.38891
H    +3.57887    +0.29526    +4.16829

* E =  +0.308 kcal/mol ; Conformer 002
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51478
C    +1.40182    +0.00000    +2.09386
C    +1.41690    -0.02513    +3.59177
C    +2.73608    +0.15808    +4.22973
O    +2.71877    -0.19054    +5.51567
C    +3.93608    +0.00779    +6.21155
O    +3.71273    +0.59967    +3.68166
H    +4.73034    -0.57842    +5.75994
H    +4.21837    +1.05582    +6.19010
H    +3.75290    -0.31706    +7.22747
H    +0.76810    +1.01165    +3.97153
H    +0.83443    -0.81319    +4.05809
H    +1.95159    -0.86904    +1.72337
H    +1.95962    +0.86969    +1.74967
H    -0.53981    +0.87328    +1.88272
H    -0.54425    -0.87145    +1.88167
H    -1.01187    +0.00318    -0.39747
H    +0.51287    +0.87678    -0.39087
```

```
H    +0.50759    -0.87946    -0.39223
H    +0.24382    +1.80992    +4.20416


* E =  +0.623 kcal/mol ; Conformer 003
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51610
C    +1.39379    +0.00000    +2.13339
C    +2.19198    +1.22661    +1.80123
C    +1.73435    +2.47858    +2.43916
O    +2.26238    +3.55590    +1.86025
C    +1.91505    +4.79317    +2.45532
O    +1.00041    +2.53816    +3.39212
H    +2.42367    +5.55328    +1.87682
H    +0.84025    +4.94167    +2.42072
H    +2.23937    +4.81969    +3.49098
H    +3.34893    +1.04787    +2.31152
H    +2.45261    +1.36535    +0.75786
H    +1.30314    -0.06887    +3.21532
H    +1.94271    -0.87839    +1.79380
H    -0.55125    +0.86035    +1.89371
H    -0.52791    -0.88216    +1.87679
H    -1.01253    -0.06565    -0.39065
H    +0.44371    +0.90672    -0.40659
H    +0.56082    -0.84696    -0.39320
H    +4.23028    +0.83538    +2.69073


* E =  +0.795 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51599
C    +1.39204    +0.00000    +2.13627
C    +2.21720    -1.19113    +1.74206
C    +3.00445    -1.06388    +0.49702
O    +3.37179    -2.25182    +0.01849
C    +4.18718    -2.21106    -1.13879
O    +3.32424    -0.02258    -0.01577
H    +3.66452    -1.71905    -1.95315
H    +5.10670    -1.67110    -0.93539
H    +4.39786    -3.24263    -1.38907
H    +3.12392    -1.31062    +2.62641
H    +1.72220    -2.15412    +1.82231
H    +1.92870    +0.90020    +1.84116
H    +1.29536    +0.02067    +3.22107
H    -0.53069    +0.87968    +1.87912
H    -0.55615    -0.86396    +1.88321
H    -1.01080    +0.09650    -0.38908
H    +0.59754    +0.82003    -0.39214
H    +0.41314    -0.92412    -0.40149
H    +3.77203    -1.37910    +3.36872
```

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*  E =   +0.846 kcal/mol ; Conformer 005
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51623
C   +1.38768   +0.00000   +2.13566
C   +2.21341   -1.19954   +1.77789
C   +3.42767   -1.41012   +2.59238
O   +4.26442   -2.27488   +2.01995
C   +5.42914   -2.57379   +2.76791
O   +3.64076   -0.90116   +3.66240
H   +6.01116   -1.67345   +2.93845
H   +5.16272   -3.00591   +3.72750
H   +5.98950   -3.28298   +2.17273
H   +1.49732   -2.22363   +2.06044
H   +2.39630   -1.36280   +0.72181
H   +1.92672   +0.89684   +1.81831
H   +1.32107   +0.05964   +3.21970
H   -0.53344   +0.87848   +1.87636
H   -0.55504   -0.86451   +1.88250
H   -1.01087   +0.08348   -0.39144
H   +0.57612   +0.83715   -0.39195
H   +0.42718   -0.91473   -0.40593
H   +0.89982   -2.97743   +2.26815
21
*  E =   +0.880 kcal/mol ; Conformer 006
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51519
C   +1.40743   +0.00000   +2.09285
C   +1.41292   +0.01902   +3.59450
C   +0.92313   -1.17352   +4.31863
O   +1.09371   -2.29848   +3.62339
C   +0.69148   -3.48326   +4.28654
O   +0.45757   -1.15603   +5.42865
H   +0.89504   -4.29269   +3.59755
H   +1.25456   -3.61199   +5.20562
H   -0.36628   -3.44218   +4.52713
H   +2.64222   +0.08479   +3.94101
H   +1.01098   +0.91690   +4.05049
H   +1.94363   -0.87929   +1.74011
H   +1.94888   +0.87329   +1.72904
H   -0.54218   +0.87094   +1.88473
H   -0.53395   -0.87672   +1.88222
H   -1.01243   -0.00132   -0.39625
H   +0.50849   +0.87884   -0.39264
H   +0.51050   -0.87836   -0.39050
H   +3.59820   +0.17536   +4.13994


*  E =   +0.913 kcal/mol ; Conformer 007
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```
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51445
C    +1.40869    +0.00000    +2.08546
C    +1.46985    +0.02949    +3.58527
C    +1.04492    +1.28399    +4.24113
O    +1.25076    +1.24438    +5.55669
C    +0.84524    +2.39972    +6.26794
O    +0.55802    +2.23314    +3.68220
H    +1.38600    +3.27194    +5.91399
H    -0.21898    +2.57048    +6.13846
H    +1.07591    +2.20395    +7.30698
H    +0.62450    -0.84607    +4.01527
H    +2.37982    -0.35956    +4.02959
H    +1.94442    -0.87991    +1.73067
H    +1.94712    +0.87004    +1.70202
H    -0.53312    +0.87207    +1.88610
H    -0.53077    -0.87866    +1.88325
H    -1.01253    -0.01430    -0.39568
H    +0.49399    +0.88796    -0.39045
H    +0.52230    -0.86976    -0.39613
H    +0.00786    -1.53926    +4.30214

* E =  +1.071 kcal/mol ; Conformer 008
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51471
C    +1.40165    +0.00000    +2.09513
C    +1.40428    -0.01349    +3.59657
C    +2.69544    +0.05377    +4.31162
O    +3.63460    +0.68855    +3.61059
C    +4.88308    +0.82857    +4.26435
O    +2.88570    -0.37623    +5.41990
H    +4.76695    +1.39274    +5.18445
H    +5.29778    -0.14618    +4.50129
H    +5.52340    +1.35734    +3.57031
H    +0.82629    +1.07262    +3.94506
H    +0.76377    -0.75798    +4.05643
H    +1.94611    -0.87545    +1.73148
H    +1.95766    +0.86651    +1.74054
H    -0.53944    +0.87332    +1.88321
H    -0.54301    -0.87161    +1.88235
H    -1.01192    +0.00100    -0.39725
H    +0.51046    +0.87803    -0.39144
H    +0.50891    -0.87867    -0.39239
H    +0.35565    +1.91470    +4.14193

* E =  +1.176 kcal/mol ; Conformer 009
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51618
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C    +1.38553    +0.00000    +2.13745
C    +2.20784    +1.20620    +1.78863
C    +3.47233    +1.35123    +2.53878
O    +4.01318    +2.55748    +2.37342
C    +5.25685    +2.75589    +3.02105
O    +3.98560    +0.48479    +3.19810
H    +5.55428    +3.76976    +2.78697
H    +5.15035    +2.62660    +4.09361
H    +5.99252    +2.04712    +2.65374
H    +2.63181    +1.06264    +0.58682
H    +1.66550    +2.14340    +1.70498
H    +1.30058    -0.04906    +3.22404
H    +1.93198    -0.89857    +1.85086
H    -0.55631    +0.86497    +1.88108
H    -0.53545    -0.87712    +1.87713
H    -1.01075    -0.09203    -0.39020
H    +0.42313    +0.91684    -0.40503
H    +0.58472    -0.83072    -0.39220
H    +2.95769    +0.91861    -0.32461

* E =  +1.408 kcal/mol ; Conformer 010
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51609
C    +1.39426    +0.00000    +2.13199
C    +2.20323    +1.21513    +1.77183
C    +1.74806    +2.53341    +2.26270
O    +1.09820    +2.44787    +3.42381
C    +0.68125    +3.68436    +3.97375
O    +1.96483    +3.58154    +1.71133
H    +0.17852    +3.44220    +4.90108
H    +1.53837    +4.32427    +4.15873
H    +0.00535    +4.19289    +3.29332
H    +3.33032    +1.06020    +2.35421
H    +2.50717    +1.29308    +0.73484
H    +1.30900    -0.06020    +3.21470
H    +1.93623    -0.88610    +1.80118
H    -0.55187    +0.86331    +1.88872
H    -0.53076    -0.87947    +1.87942
H    -1.01222    -0.06906    -0.39060
H    +0.44152    +0.90829    -0.40456
H    +0.56336    -0.84578    -0.39181
H    +4.18404    +0.86187    +2.79552

* E =  +1.552 kcal/mol ; Conformer 011
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51615
C    +1.39055    +0.00000    +2.14012
C    +2.19678    -1.22563    +1.80691
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C    +2.88557    -1.31390    +0.50150
O    +3.29783    -0.12628    +0.05945
C    +4.00557    -0.15217    -1.16651
O    +3.10149    -2.34127    -0.08866
H    +4.27445    +0.87513    -1.37569
H    +4.89355    -0.77022    -1.07850
H    +3.37774    -0.55163    -1.95707
H    +3.16699    -1.22976    +2.63206
H    +1.71204    -2.16983    +2.03118
H    +1.93882    +0.88509    +1.82292
H    +1.28908    +0.05895    +3.22325
H    -0.53094    +0.88026    +1.87777
H    -0.55692    -0.86324    +1.88278
H    -1.01156    +0.09053    -0.38835
H    +0.58571    +0.83027    -0.39012
H    +0.41828    -0.91979    -0.40484
H    +3.86474    -1.19651    +3.32861


* E =  +1.690 kcal/mol ; Conformer 012
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51637
C    +1.38734    +0.00000    +2.13816
C    +2.18314    -1.23705    +1.83107
C    +3.49388    -1.42168    +2.48830
O    +3.56277    -0.81738    +3.67423
C    +4.77937    -1.00245    +4.37517
O    +4.39736    -2.07637    +2.03586
H    +4.67286    -0.45582    +5.30316
H    +4.94746    -2.05723    +4.56894
H    +5.61231    -0.61573    +3.79645
H    +1.49020    -2.20716    +2.29545
H    +2.26153    -1.50476    +0.78435
H    +1.94305    +0.87150    +1.78108
H    +1.31332    +0.11112    +3.21753
H    -0.53249    +0.88022    +1.87393
H    -0.55682    -0.86255    +1.88480
H    -1.01202    +0.07649    -0.38979
H    +0.56903    +0.84214    -0.39111
H    +0.43324    -0.90995    -0.40923
H    +0.90140    -2.91057    +2.65448


* E =  +1.886 kcal/mol ; Conformer 013
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51602
C    +1.38622    +0.00000    +2.13747
C    +2.20601    +1.21022    +1.78178
C    +3.47126    +1.43682    +2.51143
O    +4.00636    +0.30176    +2.96033
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C    +5.24773    +0.44263    +3.62747
O    +3.99466    +2.51062    +2.65903
H    +5.54065    -0.55653    +3.92268
H    +5.98709    +0.87785    +2.96245
H    +5.13946    +1.08257    +4.49755
H    +2.62765    +1.04209    +0.58490
H    +1.65537    +2.14094    +1.69382
H    +1.29305    -0.04654    +3.22393
H    +1.93039    -0.89985    +1.85102
H    -0.55498    +0.86552    +1.88106
H    -0.53557    -0.87696    +1.87745
H    -1.01108    -0.09221    -0.38912
H    +0.42216    +0.91714    -0.40500
H    +0.58463    -0.83048    -0.39289
H    +2.95261    +0.87119    -0.32555

* E =  +2.101 kcal/mol ; Conformer 014
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51464
C    +1.39286    +0.00000    +2.13521
C    +2.24255    +1.19300    +1.78197
C    +3.15740    +1.04022    +0.62957
O    +3.92585    +2.11651    +0.46886
C    +4.81858    +2.06459    -0.62903
O    +3.21179    +0.08147    -0.09646
H    +5.50370    +1.22942    -0.52120
H    +4.26996    +1.95039    -1.55878
H    +5.35710    +3.00323    -0.61744
H    +1.46114    +2.14777    +1.41512
H    +2.74011    +1.68617    +2.60993
H    +1.29666    -0.05541    +3.21723
H    +1.92155    -0.89658    +1.80899
H    -0.55225    +0.86602    +1.88294
H    -0.53132    -0.87865    +1.87850
H    -1.01548    -0.04815    -0.38647
H    +0.45921    +0.90156    -0.40140
H    +0.55969    -0.84537    -0.39244
H    +0.85025    +2.86781    +1.16895

* E =  +2.209 kcal/mol ; Conformer 015
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51480
C    +1.39016    +0.00000    +2.13725
C    +2.35705    -1.05702    +1.67835
C    +1.93593    -2.47275    +1.67797
O    +2.97900    -3.28379    +1.49488
C    +2.66837    -4.66353    +1.43004
O    +0.80847    -2.87972    +1.79470
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H    +2.20424    -4.99170    +2.35490
H    +1.98813    -4.86110    +0.60733
H    +3.61096    -5.17223    +1.27535
H    +2.64703    -0.83059    +0.44768
H    +3.35141    -0.95050    +2.09964
H    +1.86574    +0.96451    +1.95370
H    +1.29144    -0.08164    +3.22192
H    -0.51594    +0.88839    +1.87846
H    -0.55753    -0.85964    +1.87353
H    -1.00940    +0.12300    -0.38507
H    +0.61085    +0.80659    -0.40432
H    +0.38366    -0.93873    -0.39453
H    +2.93407    -0.60232    -0.45706

* E =  +2.256 kcal/mol ; Conformer 016
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51445
C    +1.40935    +0.00000    +2.08538
C    +1.48776    +0.04923    +3.58798
C    +1.24763    +1.32412    +4.29931
O    +0.67445    +2.25268    +3.53350
C    +0.40175    +3.48260    +4.18118
O    +1.51690    +1.51063    +5.45767
H    -0.27059    +3.32750    +5.01907
H    +1.32071    +3.92909    +4.54780
H    -0.05828    +4.11578    +3.43360
H    +0.55160    -0.70992    +4.03375
H    +2.34933    -0.44024    +4.02690
H    +1.93039    -0.89320    +1.74230
H    +1.95783    +0.85276    +1.67861
H    -0.53874    +0.86892    +1.88581
H    -0.52978    -0.87872    +1.88344
H    -1.01221    -0.01820    -0.39638
H    +0.49235    +0.88851    -0.39162
H    +0.52518    -0.86832    -0.39502
H    -0.14573    -1.31970    +4.34521

* E =  +3.506 kcal/mol ; Conformer 017
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51448
C    +1.38816    +0.00000    +2.13817
C    +2.36634    -1.08035    +1.74580
C    +2.04450    -2.51948    +1.85629
O    +0.80631    -2.82001    +1.46695
C    +0.48008    -4.19816    +1.50754
O    +2.83233    -3.35687    +2.21518
H    -0.54378    -4.27022    +1.16412
H    +1.14227    -4.76254    +0.85853
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H    +0.57238    -4.57999    +2.51940
H    +2.63529    -0.92445    +0.49486
H    +3.35099    -0.92152    +2.17017
H    +1.87361    +0.95011    +1.91029
H    +1.28768    -0.02318    +3.22584
H    -0.51069    +0.89191    +1.87741
H    -0.56960    -0.85123    +1.87707
H    -1.00874    +0.12663    -0.38623
H    +0.61153    +0.80843    -0.39904
H    +0.38707    -0.93679    -0.39321
H    +2.90565    -0.74175    -0.42108


*  E =   +3.587  kcal/mol ; Conformer 018
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51428
C    +1.39217    +0.00000    +2.13665
C    +2.22250    +1.23035    +1.85025
C    +3.27718    +1.19930    +0.81197
O    +3.16928    +0.16345    -0.01870
C    +4.13490    +0.11865    -1.05353
O    +4.13416    +2.03769    +0.70008
H    +4.06713    +1.00767    -1.67265
H    +5.13493    +0.05882    -0.63561
H    +3.90897    -0.76794    -1.63178
H    +1.43797    +2.13864    +1.41174
H    +2.61227    +1.74344    +2.72142
H    +1.28941    -0.10000    +3.21517
H    +1.93315    -0.87879    +1.78611
H    -0.55191    +0.86610    +1.88242
H    -0.53311    -0.87809    +1.87690
H    -1.01598    -0.01867    -0.38749
H    +0.48899    +0.88528    -0.40168
H    +0.53014    -0.86597    -0.39013
H    +0.81662    +2.84436    +1.11352


*  E =   +3.824  kcal/mol ; Conformer 019
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51640
C    +1.40034    +0.00000    +2.12387
C    +2.07127    -1.34605    +2.22480
C    +1.69758    -2.25416    +3.33226
O    +0.53920    -1.92732    +3.90563
C    +0.12059    -2.78714    +4.95053
O    +2.34615    -3.20981    +3.67100
H    -0.82394    -2.39084    +5.30008
H    -0.00170    -3.80013    +4.58026
H    +0.85291    -2.79341    +5.75174
H    +1.76641    -2.06273    +1.19421
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H    +3.15005    -1.34095    +2.12208
H    +2.03897    +0.66609    +1.54504
H    +1.35186    +0.41624    +3.13094
H    -0.52739    +0.88593    +1.86733
H    -0.55688    -0.85379    +1.89817
H    -1.01495    -0.01070    -0.39080
H    +0.49412    +0.88951    -0.38755
H    +0.51441    -0.86642    -0.40868
H    +1.58570    -2.64696    +0.43961

* E =   +8.039 kcal/mol ; Conformer 020
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51505
C    +1.40922    +0.00000    +2.08886
C    +1.41528    +0.00905    +3.58848
C    +1.03918    -1.28073    +4.22592
O    +0.87557    -1.31069    +5.55341
C    +1.01258    -0.14553    +6.33505
O    +0.91090    -2.29614    +3.60058
H    +1.97355    +0.33692    +6.17590
H    +0.20715    +0.55936    +6.13902
H    +0.94820    -0.47410    +7.36481
H    +2.63323    +0.19102    +3.94860
H    +0.93948    +0.87999    +4.03014
H    +1.93954    -0.88374    +1.73971
H    +1.95046    +0.87433    +1.72694
H    -0.53992    +0.87429    +1.88253
H    -0.52717    -0.87812    +1.88391
H    -1.01303    +0.00138    -0.39466
H    +0.51163    +0.87611    -0.39527
H    +0.50521    -0.88212    -0.38815
H    +3.57234    +0.37848    +4.16337

* E =   +8.374 kcal/mol ; Conformer 021
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51487
C    +1.40210    +0.00000    +2.09249
C    +1.41756    -0.01864    +3.59069
C    +2.76345    +0.10063    +4.20865
O    +2.86630    -0.02463    +5.53736
C    +1.73955    -0.30911    +6.33485
O    +3.74899    +0.33325    +3.56684
H    +0.94059    +0.41090    +6.17721
H    +1.37077    -1.31678    +6.15372
H    +2.08064    -0.23967    +7.36023
H    +0.80220    +1.04858    +3.96268
H    +0.78567    -0.78199    +4.03612
H    +1.95442    -0.87011    +1.73031
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H    +1.96350    +0.86504    +1.74356
H    -0.54097    +0.87322    +1.88190
H    -0.54439    -0.87210    +1.88081
H    -1.01185    +0.00174    -0.39739
H    +0.51166    +0.87747    -0.39057
H    +0.50920    -0.87853    -0.39186
H    +0.30195    +1.86282    +4.18205


* E =   +8.703 kcal/mol ; Conformer 022
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51607
C    +1.39333    +0.00000    +2.13480
C    +2.19358    +1.22591    +1.80198
C    +1.74428    +2.47164    +2.47776
O    +2.31089    +3.63001    +2.12013
C    +3.28887    +3.68519    +1.10654
O    +0.92118    +2.47190    +3.35021
H    +4.11720    +3.01061    +1.30759
H    +2.86075    +3.46520    +0.13059
H    +3.65469    +4.70437    +1.10711
H    +3.36680    +1.02288    +2.27457
H    +2.42247    +1.34735    +0.74812
H    +1.30227    -0.06883    +3.21608
H    +1.94261    -0.87730    +1.79218
H    -0.55163    +0.85809    +1.89569
H    -0.52399    -0.88504    +1.87505
H    -1.01212    -0.07535    -0.38963
H    +0.43132    +0.91235    -0.40825
H    +0.56904    -0.84065    -0.39529
H    +4.25894    +0.79037    +2.61697


* E =   +8.859 kcal/mol ; Conformer 023
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51439
C    +1.40927    +0.00000    +2.08361
C    +1.47208    +0.04439    +3.58410
C    +1.06242    +1.33137    +4.20612
O    +1.13910    +1.44405    +5.53733
C    +1.66694    +0.40769    +6.33416
O    +0.65547    +2.26143    +3.56749
H    +1.14796    -0.53308    +6.17188
H    +2.73290    +0.27815    +6.15759
H    +1.51756    +0.72165    +7.35965
H    +0.61139    -0.82896    +4.00547
H    +2.38356    -0.36342    +4.01069
H    +1.94185    -0.88508    +1.73693
H    +1.94807    +0.86732    +1.69643
H    -0.53127    +0.87309    +1.88556
```

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H   -0.53093   -0.87885   +1.88289
H   -1.01279   -0.01597   -0.39470
H   +0.49167   +0.88937   -0.38974
H   +0.52358   -0.86867   -0.39689
H   -0.01231   -1.52466   +4.26705


* E =  +8.956 kcal/mol ; Conformer 024
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51657
C   +1.38582   +0.00000   +2.13928
C   +2.19603   -1.22030   +1.81798
C   +3.46537   -1.34594   +2.58044
O   +4.29624   -2.34840   +2.26918
C   +4.00605   -3.24041   +1.21735
O   +3.75680   -0.60584   +3.47752
H   +3.03144   -3.70607   +1.33935
H   +4.06068   -2.74365   +0.25065
H   +4.77118   -4.00539   +1.26189
H   +1.49016   -2.22389   +2.20873
H   +2.29405   -1.44030   +0.75982
H   +1.94208   +0.87790   +1.80158
H   +1.32018   +0.09430   +3.22056
H   -0.53105   +0.88110   +1.87348
H   -0.56032   -0.86071   +1.88422
H   -1.01072   +0.08595   -0.39114
H   +0.57749   +0.83632   -0.39131
H   +0.42369   -0.91513   -0.40932
H   +0.89865   -2.95037   +2.49981


* E =  +9.099 kcal/mol ; Conformer 025
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51568
C   +1.38969   +0.00000   +2.14180
C   +2.20801   -1.20287   +1.76581
C   +3.04799   -1.06396   +0.54564
O   +3.65477   -2.15692   +0.06683
C   +3.48209   -3.41895   +0.67037
O   +3.23625   -0.01190   +0.00221
H   +3.72991   -3.39790   +1.72860
H   +2.46751   -3.78809   +0.53482
H   +4.16797   -4.08365   +0.16013
H   +3.06874   -1.36279   +2.69210
H   +1.66600   -2.14243   +1.83085
H   +1.93303   +0.89314   +1.84110
H   +1.28544   +0.02829   +3.22591
H   -0.53048   +0.88004   +1.87804
H   -0.55808   -0.86267   +1.88444
H   -1.01312   +0.07901   -0.38703
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H   +0.58458   +0.82841   -0.39229
H   +0.43152   -0.91397   -0.40481
H   +3.67734   -1.46844   +3.46636


* E =  +9.208 kcal/mol ; Conformer 026
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51623
C   +1.38416   +0.00000   +2.13990
C   +2.20711   +1.20748   +1.79562
C   +3.46706   +1.33915   +2.57379
O   +4.20004   +2.44781   +2.41454
C   +3.76437   +3.50204   +1.58680
O   +3.86425   +0.47815   +3.30720
H   +3.55588   +3.16243   +0.57548
H   +2.88611   +3.99323   +2.00105
H   +4.58244   +4.21098   +1.55972
H   +2.63340   +1.05767   +0.58978
H   +1.63895   +2.12952   +1.70272
H   +1.30271   -0.04885   +3.22611
H   +1.93347   -0.89685   +1.85428
H   -0.55882   +0.86339   +1.88167
H   -0.53455   -0.87784   +1.87636
H   -1.01025   -0.09484   -0.39065
H   +0.42028   +0.91806   -0.40595
H   +0.58719   -0.82892   -0.39218
H   +2.95328   +0.90371   -0.32125


* E = +10.127 kcal/mol ; Conformer 027
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51448
C   +1.39075   +0.00000   +2.14014
C   +2.24700   +1.18801   +1.78083
C   +3.15310   +1.00789   +0.61411
O   +3.97134   +2.01623   +0.28905
C   +4.05376   +3.18330   +1.07518
O   +3.16827   +0.01214   -0.05354
H   +3.08457   +3.65872   +1.19946
H   +4.49111   +2.97293   +2.04922
H   +4.70967   +3.85438   +0.53477
H   +1.44684   +2.13905   +1.42579
H   +2.73643   +1.66678   +2.62303
H   +1.28903   -0.04367   +3.22226
H   +1.92018   -0.89838   +1.82275
H   -0.55408   +0.86502   +1.88305
H   -0.53048   -0.87898   +1.87848
H   -1.01647   -0.04244   -0.38448
H   +0.46377   +0.89851   -0.40315
H   +0.55507   -0.84754   -0.39323
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H   +0.80899   +2.84174   +1.19916
```

S.2.4 $(\mathbf{TS}_\beta)^\ddagger$

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* E =  +0.000 kcal/mol ; Conformer 001
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51521
C   +1.38055   +0.00000   +2.09723
C   +1.49182   +0.06738   +3.58898
C   +1.11459   -1.22218   +4.25998
O   +1.10300   -1.09682   +5.58413
C   +0.77706   -2.27421   +6.30265
O   +0.86143   -2.25339   +3.69840
H   +1.49460   -3.05971   +6.08746
H   +0.81254   -2.00145   +7.34925
H   -0.21508   -2.62065   +6.03105
H   +2.50958   +0.30280   +3.90105
H   +0.86330   +0.85649   +4.00056
H   +2.04331   -0.73619   +1.65070
H   +1.93407   +1.15284   +1.68156
H   -0.54752   +0.86705   +1.88957
H   -0.52764   -0.88270   +1.88496
H   -1.01268   +0.00156   -0.39477
H   +0.51308   +0.87655   -0.39061
H   +0.50580   -0.88206   -0.38754
H   +2.28871   +1.97339   +1.43506

* E =  +0.199 kcal/mol ; Conformer 002
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51550
C   +1.38170   +0.00000   +2.09568
C   +1.47616   +0.07366   +3.58687
C   +2.88504   -0.02474   +4.08755
O   +2.97909   +0.35561   +5.35885
C   +4.27428   +0.26014   +5.92577
O   +3.82360   -0.41577   +3.44940
H   +4.97349   +0.88262   +5.37656
H   +4.17664   +0.60512   +6.94681
H   +4.62391   -0.76724   +5.90076
H   +1.02936   +0.98746   +3.97598
H   +0.91930   -0.74591   +4.05122
H   +2.06025   -0.72791   +1.66102
H   +1.92358   +1.14416   +1.67691
H   -0.54935   +0.86655   +1.88766
H   -0.54169   -0.87689   +1.88340
H   -1.01231   -0.00118   -0.39577
H   +0.51039   +0.87907   -0.38732
H   +0.51169   -0.87784   -0.38941
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H    +2.23716    +1.99175    +1.43829


* E =   +0.644 kcal/mol ; Conformer 003
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51685
C    +1.36789    +0.00000    +2.13673
C    +2.35983    +1.02396    +1.67458
C    +1.99284    +2.42054    +2.08658
O    +2.79730    +3.32100    +1.52792
C    +2.54180    +4.66838    +1.88564
O    +1.10031    +2.71626    +2.83427
H    +3.27482    +5.26001    +1.35301
H    +1.53567    +4.95291    +1.59429
H    +2.64807    +4.80203    +2.95758
H    +3.34749    +0.82056    +2.08900
H    +2.48656    +1.01294    +0.59365
H    +1.34656    -0.10636    +3.21688
H    +1.91884    -1.16887    +1.76643
H    -0.54353    +0.87089    +1.89007
H    -0.54029    -0.87332    +1.88110
H    -1.01205    -0.09289    -0.38527
H    +0.41457    +0.92004    -0.40696
H    +0.58340    -0.83136    -0.39251
H    +2.29897    -1.96878    +1.48832


* E =   +0.732 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51726
C    +1.36968    +0.00000    +2.13176
C    +2.32396    +1.05801    +1.67197
C    +3.58106    +1.09900    +2.48697
O    +4.52594    +1.81886    +1.88787
C    +5.74124    +1.94200    +2.60605
O    +3.73579    +0.57675    +3.55675
H    +6.39085    +2.54692    +1.98705
H    +5.56830    +2.42308    +3.56368
H    +6.17868    +0.96375    +2.77833
H    +2.59740    +0.94131    +0.62485
H    +1.86795    +2.05054    +1.74641
H    +1.38027    -0.12992    +3.20880
H    +1.92498    -1.14710    +1.73254
H    -0.55164    +0.87198    +1.88255
H    -0.54383    -0.87004    +1.88313
H    -1.01198    -0.07510    -0.38939
H    +0.43673    +0.91116    -0.40362
H    +0.57017    -0.84234    -0.38745
H    +2.30780    -1.92944    +1.39387
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```
* E =   +0.741 kcal/mol ; Conformer 005
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.52128
C   +1.37987    +0.00000    +2.11186
C   +2.16692    -1.26722    +1.98730
C   +3.55306    -1.14673    +2.54345
O   +4.10433    -2.34065    +2.74472
C   +5.43337    -2.31947    +3.23585
O   +4.12525    -0.11503    +2.76549
H   +5.47425    -1.80761    +4.19206
H   +5.72516    -3.35583    +3.34485
H   +6.08776    -1.80925    +2.53598
H   +1.66463    -2.10286    +2.47257
H   +2.27902    -1.55903    +0.93909
H   +1.96825    +0.88543    +1.89071
H   +1.19129    +0.13852    +3.42277
H   -0.53437    +0.87954    +1.87828
H   -0.55397    -0.86553    +1.88716
H   -1.01548    +0.03399    -0.38784
H   +0.53466    +0.86356    -0.39023
H   +0.47295    -0.89308    -0.40324
H   +1.01931    +0.17343    +4.33997

* E =   +0.768 kcal/mol ; Conformer 006
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.51530
C   +1.38075    +0.00000    +2.09861
C   +1.48291    +0.07262    +3.59416
C   +0.97184    -1.14831    +4.30709
O   +1.27643    -2.27158    +3.66023
C   +0.86439    -3.46832    +4.29773
O   +0.37805    -1.13767    +5.35019
H   +1.18037    -4.27414    +3.64816
H   +1.33207    -3.55723    +5.27321
H   -0.21362    -3.47791    +4.42378
H   +2.52383    +0.19587    +3.89517
H   +0.93133    +0.91972    +3.99270
H   +2.04454    -0.73645    +1.65499
H   +1.93429    +1.14823    +1.68249
H   -0.54991    +0.86406    +1.89133
H   -0.53638    -0.88095    +1.88154
H   -1.01240    -0.00117    -0.39531
H   +0.50986    +0.87908    -0.38848
H   +0.51049    -0.87870    -0.38933
H   +2.28928    +1.96990    +1.43045

* E =   +0.825 kcal/mol ; Conformer 007
C   +0.00000    +0.00000    +0.00000
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```
C    +0.00000    +0.00000    +1.51629
C    +1.37183    +0.00000    +2.13029
C    +2.37215    +1.01783    +1.63786
C    +1.88410    +2.40253    +1.93829
O    +2.34242    +2.85549    +3.10251
C    +1.87587    +4.13930    +3.47996
O    +1.12933    +3.03003    +1.24387
H    +2.33973    +4.35435    +4.43369
H    +2.16335    +4.87843    +2.73897
H    +0.79427    +4.13711    +3.57188
H    +3.33339    +0.85761    +2.11686
H    +2.49346    +0.93923    +0.56113
H    +1.36341    -0.08854    +3.21333
H    +1.90852    -1.16170    +1.77947
H    -0.55050    +0.87442    +1.87342
H    -0.53879    -0.87008    +1.89097
H    -1.01002    -0.11684    -0.38390
H    +0.39180    +0.93568    -0.39057
H    +0.60178    -0.81878    -0.39181
H    +2.28575    -1.97540    +1.50296

* E =  +0.891 kcal/mol ; Conformer 008
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52170
C    +1.38057    +0.00000    +2.11118
C    +2.24725    -1.19122    +1.82941
C    +3.05788    -1.04299    +0.57365
O    +3.49296    -2.21956    +0.13111
C    +4.31768    -2.16743    -1.02061
O    +3.32065    -0.00324    +0.03304
H    +5.20744    -1.57819    -0.82237
H    +4.58093    -3.19333    -1.24251
H    +3.77932    -1.72202    -1.85116
H    +2.96918    -1.34200    +2.63500
H    +1.66850    -2.11076    +1.76725
H    +1.91509    +0.93731    +1.98733
H    +1.19053    -0.02827    +3.43586
H    -0.53882    +0.87405    +1.88488
H    -0.54572    -0.87298    +1.88365
H    -1.01560    +0.06194    -0.38434
H    +0.56942    +0.83849    -0.39301
H    +0.44409    -0.91109    -0.39758
H    +1.06505    -0.08629    +4.35303

* E =  +0.945 kcal/mol ; Conformer 009
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51550
C    +1.38371    +0.00000    +2.09356
```

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C    +1.50671    +0.07336    +3.59379
C    +1.08003    -1.22584    +4.21069
O    -0.16510    -1.17502    +4.67959
C    -0.64941    -2.38311    +5.24101
O    +1.75408    -2.21933    +4.25398
H    -0.02793    -2.68592    +6.07770
H    -1.65835    -2.17295    +5.57100
H    -0.64590    -3.17435    +4.49783
H    +2.54340    +0.23971    +3.87374
H    +0.89543    +0.88187    +3.98580
H    +2.04888    -0.73804    +1.65210
H    +1.93023    +1.13983    +1.67502
H    -0.54477    +0.86661    +1.89283
H    -0.54496    -0.87367    +1.88404
H    -1.01276    +0.00329    -0.39435
H    +0.51324    +0.87680    -0.38917
H    +0.50608    -0.88078    -0.39032
H    +2.28261    +1.96790    +1.42312

* E =  +1.014 kcal/mol ; Conformer 010
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51550
C    +1.38180    +0.00000    +2.09658
C    +1.46798    +0.05706    +3.59251
C    +2.84899    +0.22244    +4.15382
O    +3.77765    -0.36017    +3.40091
C    +5.10366    -0.26155    +3.89084
O    +3.10197    +0.78608    +5.18334
H    +5.18243    -0.73235    +4.86570
H    +5.72538    -0.77297    +3.16765
H    +5.39596    +0.77988    +3.97872
H    +0.86537    +0.86610    +3.99722
H    +1.06955    -0.86668    +4.02342
H    +2.05602    -0.72514    +1.65098
H    +1.92568    +1.14818    +1.68336
H    -0.54765    +0.86693    +1.88844
H    -0.54243    -0.87632    +1.88371
H    -1.01240    +0.00185    -0.39540
H    +0.51234    +0.87789    -0.38754
H    +0.50836    -0.87951    -0.39029
H    +2.26500    +1.98475    +1.44120

* E =  +1.041 kcal/mol ; Conformer 011
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51636
C    +1.37093    +0.00000    +2.13243
C    +2.36853    +1.03418    +1.67163
C    +1.93363    +2.40362    +2.10085
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O    +1.15373    +2.98513    +1.18971
C    +0.66175    +4.26653    +1.54324
O    +2.20807    +2.92075    +3.14942
H    +0.05563    +4.59242    +0.70806
H    +0.06628    +4.20712    +2.44894
H    +1.48501    +4.95391    +1.70984
H    +3.33497    +0.84208    +2.12737
H    +2.47380    +1.00987    +0.59031
H    +1.36069    -0.11036    +3.21312
H    +1.91544    -1.15343    +1.75782
H    -0.55595    +0.86930    +1.87880
H    -0.53725    -0.87261    +1.88704
H    -1.01102    -0.10416    -0.38522
H    +0.40739    +0.92703    -0.39559
H    +0.59119    -0.82718    -0.38947
H    +2.29705    -1.95867    +1.46882

* E =  +1.050 kcal/mol ; Conformer 012
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51556
C    +1.38547    +0.00000    +2.08928
C    +1.53291    +0.01174    +3.58019
C    +0.94932    +1.21735    +4.25748
O    +1.03289    +1.10470    +5.58200
C    +0.52956    +2.20642    +6.31679
O    +0.47448    +2.17558    +3.71340
H    -0.52393    +2.35558    +6.10181
H    +0.67410    +1.95750    +7.36000
H    +1.07141    +3.11149    +6.06083
H    +1.06956    -0.86990    +4.03020
H    +2.58248    -0.03513    +3.86889
H    +2.04356    -0.72883    +1.62220
H    +1.95480    +1.14997    +1.66471
H    -0.54298    +0.86497    +1.89044
H    -0.53229    -0.88421    +1.88242
H    -1.01285    -0.00917    -0.39435
H    +0.49970    +0.88600    -0.38551
H    +0.51862    -0.87224    -0.39469
H    +2.34966    +1.93447    +1.38620

* E =  +1.278 kcal/mol ; Conformer 013
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52227
C    +1.37735    +0.00000    +2.12029
C    +2.20962    -1.24163    +1.95939
C    +2.82499    -1.41138    +0.59927
O    +3.35508    -0.27788    +0.14546
C    +3.97740    -0.36611    -1.12422
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O    +2.86692    -2.44232    -0.01509
H    +4.35751    +0.62442    -1.33767
H    +4.78589    -1.08986    -1.10071
H    +3.25643    -0.66960    -1.87705
H    +3.03731    -1.22231    +2.67027
H    +1.63071    -2.13897    +2.15856
H    +1.93872    +0.91051    +1.93068
H    +1.18020    +0.08322    +3.43417
H    -0.53548    +0.87828    +1.88131
H    -0.55081    -0.86849    +1.88539
H    -1.01414    +0.08616    -0.38332
H    +0.57927    +0.83428    -0.39050
H    +0.42112    -0.91886    -0.40239
H    +1.03879    +0.11224    +4.35695

* E =  +1.492 kcal/mol ; Conformer 014
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52132
C    +1.38067    +0.00000    +2.11030
C    +2.18770    -1.25099    +1.92043
C    +3.47293    -1.30427    +2.69146
O    +4.04637    -0.10943    +2.80400
C    +5.27929    -0.09294    +3.50235
O    +3.96055    -2.30739    +3.13582
H    +5.60137    +0.94017    +3.51034
H    +5.14335    -0.45951    +4.51472
H    +6.00851    -0.71821    +2.99687
H    +1.61961    -2.13730    +2.19138
H    +2.46001    -1.36750    +0.86731
H    +1.94686    +0.90704    +1.92133
H    +1.19417    +0.08539    +3.42911
H    -0.53613    +0.87739    +1.88096
H    -0.54958    -0.86863    +1.88602
H    -1.01521    +0.03979    -0.38775
H    +0.53961    +0.86019    -0.39144
H    +0.46778    -0.89675    -0.40096
H    +1.04631    +0.10132    +4.35062

* E =  +1.629 kcal/mol ; Conformer 015
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52190
C    +1.38454    +0.00000    +2.10398
C    +2.24526    -1.21184    +1.90669
C    +1.67332    -2.48149    +2.46528
O    +2.40916    -3.53306    +2.10857
C    +1.97054    -4.78023    +2.61774
O    +0.69713    -2.57363    +3.15704
H    +0.96478    -4.99780    +2.27219
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H    +2.66995    -5.51585    +2.24248
H    +1.97352    -4.76829    +3.70317
H    +2.46311    -1.38499    +0.85072
H    +3.21793    -1.07227    +2.37853
H    +1.93361    +0.91616    +1.90049
H    +1.22253    +0.10520    +3.43991
H    -0.52559    +0.88454    +1.87973
H    -0.54881    -0.86118    +1.89574
H    -1.01590    +0.04006    -0.38626
H    +0.54016    +0.85820    -0.39618
H    +0.46442    -0.89848    -0.40204
H    +1.12452    +0.18584    +4.35087


* E =   +1.679 kcal/mol ; Conformer 016
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51727
C    +1.36733    +0.00000    +2.13959
C    +2.32002    +1.07241    +1.69933
C    +3.68643    +1.00719    +2.31460
O    +3.66162    +0.56758    +3.56975
C    +4.92128    +0.51137    +4.21646
O    +4.69786    +1.34332    +1.76162
H    +4.72704    +0.13105    +5.21081
H    +5.59205    -0.14999    +3.67755
H    +5.36609    +1.50036    +4.26409
H    +2.46695    +1.07365    +0.62349
H    +1.91315    +2.05603    +1.95672
H    +1.35918    -0.14162    +3.21495
H    +1.92915    -1.14642    +1.73634
H    -0.55575    +0.86908    +1.88311
H    -0.54141    -0.87248    +1.88127
H    -1.01113    -0.09758    -0.38651
H    +0.41452    +0.91962    -0.40652
H    +0.58718    -0.83026    -0.38792
H    +2.31920    -1.93420    +1.42104


* E =   +1.733 kcal/mol ; Conformer 017
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51547
C    +1.38289    +0.00000    +2.09496
C    +1.50853    +0.00222    +3.59300
C    +0.67574    +1.03230    +4.29827
O    +0.78500    +2.23333    +3.73933
C    +0.05296    +3.26817    +4.37136
O    +0.00214    +0.82243    +5.27053
H    +0.38292    +3.39217    +5.39805
H    +0.24967    +4.16341    +3.79618
H    -1.00780    +3.03715    +4.37008
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H   +1.22220   -0.96206   +4.01062
H   +2.54673   +0.17703   +3.87745
H   +2.04390   -0.73072   +1.63501
H   +1.95598   +1.14215   +1.65525
H   -0.54523   +0.86898   +1.88571
H   -0.54110   -0.87639   +1.88538
H   -1.01260   +0.00161   -0.39482
H   +0.51231   +0.87788   -0.38741
H   +0.50765   -0.87979   -0.39113
H   +2.35180   +1.91249   +1.34168

* E =  +1.905 kcal/mol ; Conformer 018
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.52166
C   +1.38327   +0.00000   +2.10541
C   +2.26361   -1.18649   +1.80336
C   +1.53765   -2.49100   +1.93684
O   +1.16657   -2.72314   +3.19163
C   +0.45037   -3.92663   +3.40376
O   +1.29373   -3.24319   +1.03175
H   +0.22474   -3.95406   +4.46169
H   -0.46328   -3.93194   +2.81741
H   +1.05481   -4.78196   +3.11845
H   +2.64005   -1.13934   +0.78316
H   +3.11985   -1.19121   +2.47635
H   +1.91454   +0.93848   +1.96859
H   +1.20977   +0.01131   +3.44123
H   -0.53858   +0.87109   +1.89205
H   -0.54574   -0.87315   +1.88360
H   -1.01557   +0.04857   -0.38573
H   +0.54610   +0.85623   -0.39191
H   +0.45866   -0.90466   -0.39293
H   +1.08606   +0.03422   +4.35472

* E =  +2.343 kcal/mol ; Conformer 019
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.52097
C   +1.38261   +0.00000   +2.10636
C   +2.25645   -1.20609   +1.86340
C   +1.56785   -2.48358   +2.23948
O   +0.98368   -3.06147   +1.18930
C   +0.27788   -4.25719   +1.47259
O   +1.51338   -2.94046   +3.34762
H   -0.51654   -4.06754   +2.18778
H   -0.13029   -4.59206   +0.52794
H   +0.94952   -5.00316   +1.88557
H   +2.54441   -1.25603   +0.81328
H   +3.15915   -1.13177   +2.46344
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H   +1.92541   +0.92596   +1.93394
H   +1.20619   +0.05858   +3.44089
H   -0.53270   +0.87634   +1.88809
H   -0.55295   -0.86761   +1.88301
H   -1.01525   +0.04896   -0.38700
H   +0.54631   +0.85619   -0.39178
H   +0.45945   -0.90467   -0.39111
H   +1.06801   +0.10197   +4.35246


* E =  +3.024 kcal/mol ; Conformer 020
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51826
C   +1.35691   +0.00000   +2.16548
C   +2.30022   +1.14507   +1.90687
C   +2.72782   +1.35863   +0.48468
O   +3.20284   +0.24776   -0.06664
C   +3.61680   +0.36779   -1.41514
O   +2.68196   +2.40991   -0.09618
H   +3.98725   -0.60842   -1.69946
H   +2.77668   +0.65444   -2.04126
H   +4.39621   +1.11729   -1.50879
H   +1.86044   +2.08514   +2.23915
H   +3.21043   +0.99410   +2.48717
H   +1.30420   -0.22118   +3.22777
H   +1.95002   -1.14177   +1.73159
H   -0.56393   +0.86424   +1.88268
H   -0.53782   -0.87776   +1.87513
H   -1.01109   -0.12653   -0.37885
H   +0.38027   +0.93249   -0.41020
H   +0.60981   -0.81461   -0.38533
H   +2.29610   -1.94848   +1.46465


* E =  +3.037 kcal/mol ; Conformer 021
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51634
C   +1.36119   +0.00000   +2.15314
C   +2.34794   +1.04814   +1.72437
C   +2.97906   +0.83811   +0.37705
O   +3.31932   +2.00051   -0.17952
C   +3.99058   +1.90074   -1.42318
O   +3.20277   -0.22082   -0.13934
H   +3.36132   +1.40162   -2.15340
H   +4.19852   +2.91749   -1.73006
H   +4.91224   +1.33807   -1.31230
H   +1.89530   +2.04128   +1.73421
H   +3.17777   +1.08938   +2.43031
H   +1.30941   -0.08512   +3.23434
H   +1.88818   -1.22233   +1.86229
```

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H    -0.55513    +0.87099    +1.87934
H    -0.54472    -0.87100    +1.88018
H    -1.01534    -0.07000    -0.38233
H    +0.43183    +0.91536    -0.40224
H    +0.57502    -0.83581    -0.39037
H    +2.16996    -2.07656    +1.70822


* E =   +3.988 kcal/mol ; Conformer 022
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51669
C    +1.37369    +0.00000    +2.12652
C    +2.28919    +1.16447    +1.79286
C    +3.53097    +0.73633    +1.06534
O    +3.26580    +0.39978    -0.19422
C    +4.36617    -0.10120    -0.93227
O    +4.63084    +0.67893    +1.54235
H    +3.98415    -0.32411    -1.91998
H    +5.15646    +0.64092    -0.98550
H    +4.75548    -0.99888    -0.46193
H    +1.76330    +1.88183    +1.16460
H    +2.61453    +1.67038    +2.69565
H    +1.37469    -0.23786    +3.18522
H    +1.93528    -1.10522    +1.64829
H    -0.54785    +0.87280    +1.88568
H    -0.54253    -0.87103    +1.88254
H    -1.01588    -0.01187    -0.38669
H    +0.50098    +0.87573    -0.40568
H    +0.52263    -0.87338    -0.38370
H    +2.32289    -1.88917    +1.30105


* E =   +8.033 kcal/mol ; Conformer 023
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51515
C    +1.38087    +0.00000    +2.09555
C    +1.49263    +0.06583    +3.58788
C    +1.14379    -1.24962    +4.24074
O    +1.13121    -1.29604    +5.57781
C    +1.40539    -0.15333    +6.35563
O    +0.89315    -2.24334    +3.62378
H    +0.64988    +0.61619    +6.21477
H    +1.38073    -0.48641    +7.38556
H    +2.38943    +0.25541    +6.13932
H    +2.50755    +0.33300    +3.88737
H    +0.84591    +0.84866    +3.98595
H    +2.04294    -0.73818    +1.65229
H    +1.93563    +1.15373    +1.68370
H    -0.54747    +0.86757    +1.88902
H    -0.52544    -0.88321    +1.88561
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H   -1.01298   +0.00162   -0.39377
H   +0.51314   +0.87612   -0.39160
H   +0.50470   -0.88278   -0.38700
H   +2.29541   +1.97529   +1.44566


* E =  +8.510 kcal/mol ; Conformer 024
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51554
C   +1.38252   +0.00000   +2.09372
C   +1.47642   +0.07582   +3.58510
C   +2.89624   -0.03556   +4.07600
O   +3.12112   +0.16951   +5.37946
C   +2.08174   +0.53874   +6.25555
O   +3.81535   -0.31899   +3.36642
H   +1.26354   -0.17739   +6.23807
H   +2.52076   +0.54759   +7.24533
H   +1.70413   +1.53309   +6.02780
H   +1.02797   +1.00101   +3.94942
H   +0.89783   -0.73055   +4.04781
H   +2.06471   -0.72342   +1.65917
H   +1.92038   +1.14844   +1.68114
H   -0.54948   +0.86717   +1.88689
H   -0.54239   -0.87683   +1.88284
H   -1.01229   -0.00081   -0.39566
H   +0.51090   +0.87879   -0.38712
H   +0.51147   -0.87795   -0.38909
H   +2.21714   +2.00259   +1.45221


* E =  +8.672 kcal/mol ; Conformer 025
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51668
C   +1.36736   +0.00000   +2.13722
C   +2.36703   +1.01209   +1.66409
C   +2.00921   +2.41276   +2.09662
O   +2.78340   +3.41452   +1.66284
C   +3.88197   +3.17904   +0.81227
O   +1.08303   +2.66430   +2.81085
H   +3.56316   +2.79922   -0.15575
H   +4.35749   +4.14181   +0.67325
H   +4.59721   +2.49192   +1.25772
H   +3.35607   +0.77859   +2.06170
H   +2.46987   +0.98383   +0.57973
H   +1.34600   -0.09029   +3.21855
H   +1.91486   -1.17313   +1.77901
H   -0.54297   +0.87018   +1.89043
H   -0.53775   -0.87491   +1.88071
H   -1.01095   -0.10492   -0.38471
H   +0.39983   +0.92698   -0.40656
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H    +0.59311   -0.82387   -0.39438
H    +2.29996   -1.97462   +1.50741


* E =  +9.052 kcal/mol ; Conformer 026
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.51735
C    +1.36880   +0.00000   +2.13370
C    +2.32283   +1.05742   +1.67085
C    +3.57794   +1.09650   +2.50328
O    +4.56500   +1.90525   +2.09887
C    +4.46557   +2.64900   +0.90685
O    +3.72266   +0.46381   +3.50701
H    +3.58535   +3.28757   +0.89999
H    +5.35160   +3.27057   +0.87356
H    +4.45580   +2.00106   +0.03319
H    +2.58461   +0.91495   +0.62218
H    +1.85477   +2.04662   +1.72211
H    +1.38307   -0.13217   +3.20963
H    +1.92825   -1.14354   +1.72970
H    -0.55417   +0.87029   +1.88291
H    -0.54250   -0.87113   +1.88227
H    -1.01133   -0.08081   -0.38975
H    +0.43049   +0.91417   -0.40440
H    +0.57475   -0.83917   -0.38766
H    +2.31084   -1.91737   +1.37643


* E =  +9.063 kcal/mol ; Conformer 027
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.52129
C    +1.37935   +0.00000   +2.11300
C    +2.15947   -1.27285   +2.00005
C    +3.55906   -1.13412   +2.53972
O    +4.29830   -2.24528   +2.64352
C    +3.77254   -3.51111   +2.31911
O    +4.04112   -0.08588   +2.85189
H    +3.38753   -3.54145   +1.30250
H    +4.60071   -4.20367   +2.40269
H    +2.99211   -3.80816   +3.01619
H    +1.63994   -2.08358   +2.51265
H    +2.23909   -1.59089   +0.95575
H    +1.97279   +0.88076   +1.89050
H    +1.19014   +0.14177   +3.42379
H    -0.53287   +0.88073   +1.87740
H    -0.55688   -0.86362   +1.88791
H    -1.01532   +0.03407   -0.38813
H    +0.53477   +0.86349   -0.38988
H    +0.47286   -0.89279   -0.40455
H    +1.00734   +0.16875   +4.33699
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* E =  +9.089 kcal/mol ; Conformer 028
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.52135
C   +1.37863   +0.00000   +2.11560
C   +2.23967   -1.20071   +1.85415
C   +3.11640   -1.03332   +0.63676
O   +3.81678   -2.09744   +0.22657
C   +3.71963   -3.34119   +0.88197
O   +3.23197   -0.00141   +0.04349
H   +2.73201   -3.78010   +0.75944
H   +4.45071   -3.98196   +0.40516
H   +3.95613   -3.26037   +1.94006
H   +2.90203   -1.38876   +2.70308
H   +1.62872   -2.09761   +1.75018
H   +1.91935   +0.93180   +1.98289
H   +1.18263   -0.01615   +3.43559
H   -0.53845   +0.87434   +1.88429
H   -0.54718   -0.87187   +1.88498
H   -1.01726   +0.04616   -0.38217
H   +0.55766   +0.84571   -0.39271
H   +0.46111   -0.90103   -0.40027
H   +1.05722   -0.07166   +4.35635

* E =  +9.346 kcal/mol ; Conformer 029
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51637
C   +1.37218   +0.00000   +2.13013
C   +2.35695   +1.04275   +1.65504
C   +1.82677   +2.42343   +1.94930
O   +2.10845   +2.98885   +3.12856
C   +2.99564   +2.38785   +4.04382
O   +1.11074   +3.00493   +1.18586
H   +4.01254   +2.37491   +3.65848
H   +2.96391   +3.00635   +4.93218
H   +2.68695   +1.37863   +4.30430
H   +3.33159   +0.87011   +2.10254
H   +2.46677   +0.98442   +0.57651
H   +1.35664   -0.11975   +3.21092
H   +1.92355   -1.14504   +1.75649
H   -0.54990   +0.87426   +1.87424
H   -0.53662   -0.87117   +1.89115
H   -1.01056   -0.11815   -0.38178
H   +0.38895   +0.93664   -0.39039
H   +0.60168   -0.81872   -0.39217
H   +2.31655   -1.94898   +1.46604

* E =  +9.346 kcal/mol ; Conformer 030
```

```
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51513
C    +1.38456    +0.00000    +2.09114
C    +1.49892    +0.04159    +3.59606
C    +1.00682    -1.25560    +4.18707
O    +1.87373    -2.26349    +4.34278
C    +3.25309    -2.09829    +4.10612
O    -0.14318    -1.43434    +4.46651
H    +3.70129    -1.42551    +4.83367
H    +3.69014    -3.08242    +4.22137
H    +3.45272    -1.73838    +3.09997
H    +2.51972    +0.26547    +3.89404
H    +0.85094    +0.81958    +3.98896
H    +2.05027    -0.72046    +1.61868
H    +1.92386    +1.14243    +1.70092
H    -0.53949    +0.86946    +1.89273
H    -0.54461    -0.86822    +1.89292
H    -1.01359    +0.00831    -0.39158
H    +0.51678    +0.87363    -0.39234
H    +0.49828    -0.88481    -0.39204
H    +2.27964    +1.98203    +1.46358

* E =  +9.498 kcal/mol ; Conformer 031
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51558
C    +1.38628    +0.00000    +2.08668
C    +1.53773    +0.00716    +3.57845
C    +0.97026    +1.23348    +4.24827
O    +1.01532    +1.27703    +5.58689
C    +1.55882    +0.22246    +6.34563
O    +0.49815    +2.15899    +3.65821
H    +2.59820    +0.03295    +6.08792
H    +1.50634    +0.54599    +7.37770
H    +0.98097    -0.69224    +6.23310
H    +1.06094    -0.87735    +4.01128
H    +2.59104    -0.06726    +3.85097
H    +2.04178    -0.73151    +1.61982
H    +1.96268    +1.14972    +1.66051
H    -0.54275    +0.86399    +1.89156
H    -0.53078    -0.88576    +1.88167
H    -1.01314    -0.01179    -0.39329
H    +0.49629    +0.88796    -0.38519
H    +0.52088    -0.87046    -0.39582
H    +2.36591    +1.92474    +1.37830

* E = +10.008 kcal/mol ; Conformer 032
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52084
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```
C   +1.38534   +0.00000   +2.10085
C   +2.28688   -1.17872   +1.80785
C   +1.61995   -2.49963   +2.09548
O   +1.86523   -3.12387   +3.24924
C   +2.80383   -2.63337   +4.18153
O   +0.84838   -2.99356   +1.32331
H   +2.57514   -1.61606   +4.48566
H   +2.72633   -3.28575   +5.04241
H   +3.81575   -2.68909   +3.78640
H   +2.50899   -1.19341   +0.74085
H   +3.23058   -1.06243   +2.33215
H   +1.91424   +0.93875   +1.95410
H   +1.19711   +0.03679   +3.43022
H   -0.52367   +0.88030   +1.89144
H   -0.55138   -0.86921   +1.87523
H   -1.01444   +0.08675   -0.38135
H   +0.57725   +0.83364   -0.39721
H   +0.41658   -0.92758   -0.38390
H   +1.02995   +0.07998   +4.34490


* E = +10.061 kcal/mol ; Conformer 033
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.52190
C   +1.38441   +0.00000   +2.10392
C   +2.25285   -1.20678   +1.89982
C   +1.69187   -2.47539   +2.49018
O   +2.37872   -3.60669   +2.27896
C   +3.57171   -3.62125   +1.53082
O   +0.68792   -2.52440   +3.13639
H   +4.32411   -2.96158   +1.95660
H   +3.93332   -4.64104   +1.57451
H   +3.39633   -3.35368   +0.49110
H   +2.44228   -1.36914   +0.83533
H   +3.23497   -1.03716   +2.34311
H   +1.93139   +0.91768   +1.90085
H   +1.22786   +0.10140   +3.44385
H   -0.52169   +0.88715   +1.87881
H   -0.54997   -0.85919   +1.89651
H   -1.01577   +0.04826   -0.38530
H   +0.54720   +0.85309   -0.39791
H   +0.45389   -0.90386   -0.40261
H   +1.13776   +0.18315   +4.35258


* E = +10.120 kcal/mol ; Conformer 034
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51531
C   +1.38700   +0.00000   +2.08598
C   +1.52969   -0.01208   +3.59070
```

```
C    +0.85117    +1.17148    +4.23430
O    +1.57865    +2.24217    +4.56308
C    +2.98203    +2.26724    +4.42478
O    -0.32976    +1.19203    +4.43135
H    +3.29066    +2.05657    +3.40477
H    +3.28154    +3.27552    +4.68252
H    +3.45720    +1.57113    +5.11255
H    +1.01846    -0.89050    +3.98456
H    +2.57634    -0.08993    +3.86719
H    +2.04981    -0.72076    +1.61280
H    +1.91863    +1.15232    +1.65046
H    -0.55576    +0.85469    +1.89666
H    -0.53017    -0.88039    +1.88953
H    -1.01385    -0.00575    -0.39099
H    +0.50141    +0.88351    -0.38990
H    +0.51352    -0.87474    -0.39544
H    +2.23756    +1.97310    +1.33690

* E = +10.511 kcal/mol ; Conformer 035
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52132
C    +1.38443    +0.00000    +2.11437
C    +1.99930    -1.33709    +2.46131
C    +2.02328    -2.26095    +1.27006
O    +3.04238    -2.17874    +0.40705
C    +4.16906    -1.37417    +0.67142
O    +1.13172    -3.02617    +1.04066
H    +4.73654    -1.75675    +1.51665
H    +4.78391    -1.42820    -0.21836
H    +3.89446    -0.33800    +0.84938
H    +2.98942    -1.19779    +2.88754
H    +1.37812    -1.83419    +3.20095
H    +2.06320    +0.68147    +1.60530
H    +1.28360    +0.58132    +3.28054
H    -0.53180    +0.88456    +1.87283
H    -0.55065    -0.86475    +1.88926
H    -1.01804    +0.02974    -0.38104
H    +0.52356    +0.87238    -0.38754
H    +0.47280    -0.89012    -0.40567
H    +1.18591    +0.97961    +4.13904

* E = +10.782 kcal/mol ; Conformer 036
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52083
C    +1.38674    +0.00000    +2.09749
C    +2.21115    -1.25527    +1.88505
C    +3.25198    -1.05442    +0.81590
O    +4.34896    -0.35582    +1.13667
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```
C    +4.65590    -0.03876    +2.47661
O    +3.12066    -1.44323    -0.30785
H    +4.89696    -0.93451    +3.04463
H    +5.53162    +0.59685    +2.43390
H    +3.85035    +0.49979    +2.96900
H    +2.68075    -1.56567    +2.81842
H    +1.57527    -2.06985    +1.55262
H    +1.93101    +0.91959    +1.88994
H    +1.23366    +0.09317    +3.39816
H    -0.53727    +0.87275    +1.89012
H    -0.53686    -0.87511    +1.88873
H    -1.01767    -0.00844    -0.38321
H    +0.49670    +0.88609    -0.38987
H    +0.52107    -0.86625    -0.40013
H    +1.15186    +0.11614    +4.34107

* E = +10.887 kcal/mol ; Conformer 037
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51539
C    +1.38264    +0.00000    +2.09619
C    +1.46511    +0.07589    +3.59992
C    +2.89111    +0.07413    +4.08247
O    +3.52882    -1.10171    +4.17393
C    +2.84362    -2.32613    +4.04664
O    +3.48803    +1.07671    +4.34056
H    +2.30434    -2.39784    +3.10550
H    +3.60629    -3.09448    +4.07550
H    +2.15647    -2.48000    +4.87596
H    +1.02334    +1.00650    +3.94491
H    +0.89556    -0.74121    +4.04665
H    +2.04867    -0.73101    +1.64267
H    +1.92127    +1.14877    +1.66671
H    -0.54175    +0.87033    +1.88865
H    -0.54556    -0.87349    +1.88538
H    -1.01274    +0.00502    -0.39411
H    +0.51458    +0.87639    -0.38735
H    +0.50476    -0.88112    -0.39162
H    +2.22564    +1.98126    +1.38841

* E = +11.287 kcal/mol ; Conformer 038
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.52073
C    +1.38424    +0.00000    +2.10310
C    +2.12941    -1.31261    +2.04788
C    +3.57787    -1.14284    +2.41461
O    +4.40702    -0.64915    +1.48281
C    +4.01297    -0.52853    +0.13515
O    +4.00693    -1.37769    +3.50497
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```
H    +3.10643    +0.06166    +0.02259
H    +4.82895    -0.02282    -0.36618
H    +3.87093    -1.50650    -0.32021
H    +1.70297    -2.01002    +2.76378
H    +2.03071    -1.76216    +1.05857
H    +1.97590    +0.86512    +1.81082
H    +1.21240    +0.23895    +3.40460
H    -0.53559    +0.87820    +1.87943
H    -0.54703    -0.86747    +1.89094
H    -1.01471    -0.00329    -0.39075
H    +0.50097    +0.88459    -0.38954
H    +0.50603    -0.87533    -0.40384
H    +1.03248    +0.37217    +4.30631


* E = +11.392 kcal/mol ; Conformer 039
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51670
C    +1.37378    +0.00000    +2.12499
C    +2.33079    +1.06058    +1.63641
C    +3.61011    +1.05418    +2.42838
O    +3.61611    +1.65728    +3.62622
C    +2.54617    +2.47073    +4.04872
O    +4.59988    +0.49630    +2.05778
H    +1.59686    +1.94129    +4.02997
H    +2.77428    +2.75015    +5.06988
H    +2.47523    +3.37220    +3.44379
H    +2.60832    +0.87080    +0.60393
H    +1.85023    +2.04084    +1.66988
H    +1.36890    -0.13016    +3.20410
H    +1.91474    -1.16123    +1.73412
H    -0.55258    +0.87117    +1.88246
H    -0.53958    -0.87235    +1.88377
H    -1.01251    -0.07562    -0.38731
H    +0.43558    +0.91143    -0.40371
H    +0.57052    -0.84183    -0.38735
H    +2.25522    -1.96594    +1.41696


* E = +11.590 kcal/mol ; Conformer 040
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.51610
C    +1.38451    +0.00000    +2.09327
C    +1.52899    +0.12957    +3.58910
C    +0.81643    +1.35647    +4.10642
O    -0.34709    +1.22286    +4.75575
C    -0.91342    -0.03568    +5.03823
O    +1.25024    +2.45611    +3.92872
H    -0.29371    -0.60615    +5.72640
H    -1.86437    +0.17284    +5.51302
```

```
H   -1.08939   -0.61160   +4.13350
H   +1.19544   -0.78409   +4.07911
H   +2.57813   +0.26626   +3.83850
H   +2.02242   -0.78168   +1.68856
H   +1.98506   +1.09797   +1.58043
H   -0.55127   +0.86715   +1.88464
H   -0.54060   -0.88231   +1.87490
H   -1.01275   -0.01119   -0.39384
H   +0.50075   +0.88463   -0.38576
H   +0.51927   -0.87322   -0.39044
H   +2.39097   +1.84543   +1.22882


* E = +11.703 kcal/mol ; Conformer 041
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51626
C   +1.37409   +0.00000   +2.12682
C   +2.29708   +1.13941   +1.73095
C   +3.27163   +0.78225   +0.63197
O   +4.34445   +0.05328   +0.95735
C   +4.64607   -0.25965   +2.29771
O   +3.11758   +1.11023   -0.50788
H   +3.81575   -0.74917   +2.79954
H   +5.48385   -0.94460   +2.25768
H   +4.94294   +0.62950   +2.85018
H   +1.71391   +1.97054   +1.34197
H   +2.84382   +1.49869   +2.59946
H   +1.36246   -0.18383   +3.19739
H   +1.90208   -1.13434   +1.68750
H   -0.54081   +0.87687   +1.88537
H   -0.54444   -0.86737   +1.88842
H   -1.01670   -0.00975   -0.38415
H   +0.50575   +0.87200   -0.40651
H   +0.51411   -0.87761   -0.38662
H   +2.24184   -1.94871   +1.34785


* E = +11.818 kcal/mol ; Conformer 042
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.51573
C   +1.35541   +0.00000   +2.16542
C   +2.33837   +1.06354   +1.76440
C   +3.10212   +0.80218   +0.48825
O   +3.87925   +1.79635   +0.03234
C   +3.95904   +3.04156   +0.68474
O   +3.07857   -0.22827   -0.11370
H   +4.26536   +2.93728   +1.72292
H   +4.71452   +3.60458   +0.15070
H   +3.01608   +3.58170   +0.63375
H   +1.82665   +2.02630   +1.67489
```

```
H   +3.08119   +1.20194   +2.55076
H   +1.28679   -0.09082   +3.24531
H   +1.89535   -1.22134   +1.88304
H   -0.55399   +0.87258   +1.87875
H   -0.54890   -0.86832   +1.87950
H   -1.01877   -0.02916   -0.37885
H   +0.47199   +0.89334   -0.40520
H   +0.54359   -0.85489   -0.39111
H   +2.18789   -2.07210   +1.74927


* E = +11.921 kcal/mol ; Conformer 043
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.52084
C   +1.36876   +0.00000   +2.15009
C   +2.12786   +1.30676   +2.27198
C   +1.85563   +2.29082   +1.16390
O   +2.66803   +2.33776   +0.10571
C   +3.80205   +1.50364   +0.00559
O   +0.90897   +3.02435   +1.19856
H   +3.54181   +0.45557   +0.12193
H   +4.19563   +1.66430   -0.99039
H   +4.56036   +1.78289   +0.73367
H   +1.78479   +1.81267   +3.17297
H   +3.18972   +1.10748   +2.39900
H   +1.41292   -0.53776   +3.09275
H   +2.11666   -0.83603   +1.41159
H   -0.54923   +0.87372   +1.87932
H   -0.53988   -0.87662   +1.87323
H   -1.01921   +0.00094   -0.37737
H   +0.49377   +0.87406   -0.41537
H   +0.49905   -0.88671   -0.38509
H   +2.64991   -1.43551   +0.93788
```

S.2.5 $(\mathbf{TS}_\gamma)^\ddagger$

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* E =  +0.000 kcal/mol ; Conformer 001
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49651
C   +1.34289   +0.00000   +2.16491
C   +1.26090   +0.08482   +3.67441
C   +0.71693   -1.16383   +4.29796
O   +0.47557   -0.99915   +5.59571
C   -0.01280   -2.14328   +6.27366
O   +0.52923   -2.20439   +3.72632
H   -0.15234   -1.84028   +7.30312
H   -0.95355   -2.46745   +5.83995
H   +0.70277   -2.95692   +6.20806
H   +2.24495   +0.25055   +4.11240
```

```
H   +0.64592   +0.92449   +3.99440
H   +1.87984   -0.91005   +1.88761
H   +1.93165   +0.83859   +1.79274
H   -0.53919   +1.17068   +1.84548
H   -0.69787   -0.70750   +1.93547
H   -1.00557   +0.10633   -0.39880
H   +0.60804   +0.81231   -0.39456
H   +0.41014   -0.93477   -0.38562
H   -0.86351   +2.02041   +2.07097

* E =   +0.293 kcal/mol ; Conformer 002
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49713
C   +1.34067   +0.00000   +2.16764
C   +1.23658   +0.09676   +3.67336
C   +2.57299   +0.08202   +4.34541
O   +2.45858   +0.18568   +5.66762
C   +3.68006   +0.17967   +6.38500
O   +3.63246   -0.01216   +3.78705
H   +3.41081   +0.27109   +7.42920
H   +4.21865   -0.74621   +6.20873
H   +4.30434   +1.01256   +6.07699
H   +0.71904   +1.00706   +3.97468
H   +0.65046   -0.72521   +4.08475
H   +1.88995   -0.90601   +1.90083
H   +1.94360   +0.82578   +1.79076
H   -0.54783   +1.16238   +1.84532
H   -0.70671   -0.70202   +1.93526
H   -1.00614   +0.09764   -0.39954
H   +0.60078   +0.81879   -0.39106
H   +0.42145   -0.92839   -0.38901
H   -0.88808   +2.00819   +2.07169

* E =   +0.805 kcal/mol ; Conformer 003
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49845
C   +1.33540   +0.00000   +2.18730
C   +2.12841   -1.27781   +1.97014
C   +1.49682   -2.47076   +2.61965
O   +2.04773   -3.60750   +2.20058
C   +1.53919   -4.78643   +2.80003
O   +0.61631   -2.43476   +3.43632
H   +2.08875   -5.60567   +2.35517
H   +1.69268   -4.76160   +3.87434
H   +0.47696   -4.88497   +2.59974
H   +2.27563   -1.49674   +0.91457
H   +3.12857   -1.18436   +2.39487
H   +1.93016   +0.83822   +1.82404
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H    +1.19067    +0.14334    +3.25611
H    -0.53305    +1.17009    +1.83534
H    -0.70930    -0.69063    +1.94469
H    -1.00061    +0.16069    -0.39384
H    +0.64655    +0.78275    -0.39394
H    +0.35346    -0.95082    -0.40283
H    -0.86784    +2.01808    +2.04675


* E =   +0.924 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49831
C    +1.32160    +0.00000    +2.21547
C    +2.28389    +1.06997    +1.73430
C    +3.03779    +0.67350    +0.50152
O    +3.52534    +1.73179    -0.14050
C    +4.30443    +1.44110    -1.28776
O    +3.22341    -0.45516    +0.13241
H    +4.62197    +2.39833    -1.68016
H    +5.16303    +0.83382    -1.01883
H    +3.71137    +0.90463    -2.02170
H    +1.78224    +2.01889    +1.55500
H    +3.04121    +1.26725    +2.49353
H    +1.14178    +0.13552    +3.28047
H    +1.80177    -0.97365    +2.09738
H    -0.55738    +1.15508    +1.84575
H    -0.70389    -0.70674    +1.92954
H    -1.01493    +0.01113    -0.38873
H    +0.51350    +0.87231    -0.40275
H    +0.50705    -0.88288    -0.39028
H    -0.90700    +1.99456    +2.09121


* E =   +0.951 kcal/mol ; Conformer 005
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49881
C    +1.32475    +0.00000    +2.20636
C    +2.23144    +1.13843    +1.78942
C    +3.49501    +1.18248    +2.58952
O    +4.28350    +2.18382    +2.20478
C    +5.50325    +2.30328    +2.91509
O    +3.78833    +0.42337    +3.47310
H    +6.01484    +3.15407    +2.48424
H    +5.31229    +2.46683    +3.97108
H    +6.09772    +1.40210    +2.80172
H    +2.51342    +1.07420    +0.73957
H    +1.73029    +2.09997    +1.90369
H    +1.16768    +0.04858    +3.28200
H    +1.83661    -0.94927    +2.02890
H    -0.56974    +1.15521    +1.84898
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H   -0.69993   -0.71121   +1.92828
H   -1.01314   -0.00505   -0.39309
H   +0.50641   +0.87326   -0.40609
H   +0.50931   -0.88399   -0.38930
H   -0.93124   +1.98751   +2.08389


* E =  +1.021 kcal/mol ; Conformer 006
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49849
C   +1.33284   +0.00000   +2.18971
C   +2.07721   -1.30991   +2.00878
C   +3.39287   -1.32629   +2.72329
O   +4.02744   -2.48451   +2.55300
C   +5.28479   -2.58789   +3.19791
O   +3.84357   -0.42395   +3.37481
H   +5.65866   -3.57558   +2.96154
H   +5.96298   -1.82426   +2.83020
H   +5.17109   -2.46877   +4.27084
H   +1.49127   -2.15307   +2.37494
H   +2.27297   -1.52062   +0.95805
H   +1.94863   +0.81472   +1.81052
H   +1.20446   +0.18844   +3.25385
H   -0.55132   +1.16198   +1.84025
H   -0.71307   -0.69724   +1.93353
H   -0.99976   +0.16128   -0.39584
H   +0.64741   +0.78355   -0.38992
H   +0.35583   -0.95036   -0.40149
H   -0.91409   +1.99407   +2.06294


* E =  +1.196 kcal/mol ; Conformer 007
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49769
C   +1.34742   +0.00000   +2.15885
C   +1.28529   -0.06551   +3.67742
C   +0.61449   +1.12572   +4.29065
O   +1.19474   +2.26285   +3.91372
C   +0.59215   +3.44364   +4.41224
O   -0.32512   +1.08727   +5.03756
H   +1.17455   +4.26479   +4.01491
H   -0.43798   +3.50747   +4.07493
H   +0.61073   +3.44967   +5.49754
H   +0.74229   -0.94453   +4.01109
H   +2.29500   -0.11935   +4.08182
H   +1.91695   -0.86214   +1.80110
H   +1.90656   +0.88449   +1.85457
H   -0.57589   +1.16089   +1.81911
H   -0.70059   -0.70556   +1.93877
H   -1.00591   +0.10335   -0.39840
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H   +0.60373   +0.81656   -0.39172
H   +0.41558   -0.93089   -0.38939
H   -0.97060   +1.99576   +1.97502


* E =  +1.228 kcal/mol ; Conformer 008
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49699
C   +1.34324   +0.00000   +2.16680
C   +1.27075   +0.22908   +3.66592
C   +1.07008   +1.67689   +4.00192
O   +0.29069   +1.84422   +5.06533
C   +0.07775   +3.19111   +5.45102
O   +1.57386   +2.59175   +3.40828
H   -0.57078   +3.15228   +6.31650
H   +1.02073   +3.66799   +5.69938
H   -0.39340   +3.74157   +4.64278
H   +0.48650   -0.36249   +4.13107
H   +2.21009   -0.06134   +4.13642
H   +1.82902   -0.96031   +1.97574
H   +1.97976   +0.76650   +1.72688
H   -0.60530   +1.14735   +1.83783
H   -0.69418   -0.71465   +1.93507
H   -1.00849   +0.07345   -0.39891
H   +0.58035   +0.83384   -0.38964
H   +0.44261   -0.91836   -0.39041
H   -1.05185   +1.94071   +2.04107


* E =  +1.271 kcal/mol ; Conformer 009
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49684
C   +1.34206   +0.00000   +2.16650
C   +1.25435   +0.04837   +3.68083
C   +0.59461   -1.14004   +4.31380
O   +0.84360   -2.27155   +3.65479
C   +0.28627   -3.44091   +4.22817
O   -0.06139   -1.10725   +5.31911
H   +0.57407   -4.25674   +3.57783
H   +0.67600   -3.59386   +5.22965
H   -0.79462   -3.35749   +4.28277
H   +2.25425   +0.10827   +4.11140
H   +0.71160   +0.92594   +4.02063
H   +1.89844   -0.88937   +1.86366
H   +1.91728   +0.85895   +1.81963
H   -0.54288   +1.16789   +1.84444
H   -0.70379   -0.70514   +1.93393
H   -1.00558   +0.10434   -0.39915
H   +0.60503   +0.81557   -0.39209
H   +0.41495   -0.93157   -0.38833
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H    -0.86933    +2.01869    +2.05912


* E =   +1.317 kcal/mol ; Conformer 010
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49886
C    +1.32758    +0.00000    +2.20665
C    +2.33992    +0.99771    +1.65539
C    +1.82772    +2.40399    +1.69927
O    +1.63487    +2.81714    +2.94880
C    +1.08495    +4.11625    +3.07946
O    +1.59597    +3.08940    +0.73965
H    +0.98897    +4.29203    +4.14301
H    +1.74155    +4.85240    +2.62643
H    +0.11419    +4.16039    +2.59520
H    +3.25192    +0.94569    +2.24648
H    +2.59082    +0.77771    +0.62291
H    +1.17384    +0.19437    +3.26693
H    +1.76781    -0.99810    +2.13572
H    -0.60921    +1.13533    +1.85091
H    -0.69172    -0.71607    +1.93474
H    -1.01429    -0.02651    -0.38886
H    +0.48688    +0.88660    -0.40031
H    +0.52514    -0.87504    -0.38960
H    -1.04954    +1.92651    +2.09322


* E =   +1.335 kcal/mol ; Conformer 011
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49821
C    +1.32546    +0.00000    +2.20640
C    +2.11574    -1.28618    +2.00875
C    +2.83837    -1.33792    +0.69695
O    +3.04303    -2.58925    +0.29269
C    +3.78343    -2.72555    -0.90799
O    +3.22888    -0.38217    +0.08250
H    +3.86165    -3.78970    -1.08839
H    +3.26808    -2.23515    -1.72779
H    +4.76821    -2.28244    -0.79788
H    +2.88944    -1.36947    +2.77344
H    +1.49226    -2.17178    +2.10775
H    +1.93339    +0.83304    +1.85602
H    +1.15879    +0.14562    +3.27202
H    -0.55020    +1.15790    +1.84685
H    -0.71330    -0.69917    +1.93065
H    -0.99686    +0.19276    -0.38994
H    +0.68134    +0.75028    -0.39347
H    +0.31799    -0.96583    -0.39802
H    -0.91391    +1.98810    +2.08550
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* E =  +1.335 kcal/mol ; Conformer 012
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49705
C   +1.34098    +0.00000    +2.16790
C   +1.22892    +0.08837    +3.68063
C   +2.54467    +0.07046    +4.39345
O   +3.42872    +0.89515    +3.83389
C   +4.69121    +0.95566    +4.47342
O   +2.79604    -0.58606    +5.36749
H   +5.28081    +1.65910    +3.90001
H   +4.58016    +1.29556    +5.49835
H   +5.16052    -0.02306    +4.47805
H   +0.72452    +1.01685    +3.95115
H   +0.64063    -0.73034    +4.08411
H   +1.88103    -0.91118    +1.89357
H   +1.93992    +0.83054    +1.79726
H   -0.54374    +1.16526    +1.84622
H   -0.70615    -0.70123    +1.93650
H   -1.00620    +0.10034    -0.39867
H   +0.60223    +0.81750    -0.39167
H   +0.41765    -0.92986    -0.38979
H   -0.88039    +2.01175    +2.07017

* E =  +1.456 kcal/mol ; Conformer 013
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49716
C   +1.34117    +0.00000    +2.16747
C   +1.23145    +0.09567    +3.67984
C   +2.54742    +0.08280    +4.39318
O   +3.36323    -0.86086    +3.92366
C   +4.61930    -0.95324    +4.57206
O   +2.85172    +0.81012    +5.29905
H   +5.15242    -1.75260    +4.07393
H   +5.16138    -0.01721    +4.48195
H   +4.48577    -1.18035    +5.62513
H   +0.71350    +1.00067    +3.98187
H   +0.65509    -0.75041    +4.05744
H   +1.88688    -0.90742    +1.90136
H   +1.93413    +0.83345    +1.78752
H   -0.55179    +1.16256    +1.84383
H   -0.70278    -0.70482    +1.93680
H   -1.00667    +0.09547    -0.39865
H   +0.59733    +0.82122    -0.39156
H   +0.42316    -0.92718    -0.39010
H   -0.89658    +2.00645    +2.06204

* E =  +1.461 kcal/mol ; Conformer 014
C   +0.00000    +0.00000    +0.00000
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C   +0.00000    +0.00000    +1.49783
C   +1.33670    +0.00000    +2.18444
C   +2.18775    -1.21975    +1.82821
C   +1.46575    -2.50208    +2.09972
O   +1.18279    -2.64478    +3.39334
C   +0.47803    -3.82508    +3.73558
O   +1.14871    -3.31203    +1.27046
H   +0.32945    -3.78211    +4.80665
H   -0.47559    -3.86032    +3.21810
H   +1.05614    -4.70288    +3.46449
H   +2.45282    -1.21927    +0.77602
H   +3.10521    -1.20639    +2.41382
H   +1.89352    +0.89341    +1.90168
H   +1.19764    +0.03422    +3.26281
H   -0.55085    +1.15859    +1.85538
H   -0.70713    -0.70477    +1.93028
H   -0.99554    +0.18839    -0.39413
H   +0.66927    +0.76346    -0.39364
H   +0.32608    -0.96574    -0.38914
H   -0.90347    +1.99290    +2.08324

* E =  +1.571 kcal/mol ; Conformer 015
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49877
C   +1.32772    +0.00000    +2.20547
C   +2.31528    +1.05596    +1.71948
C   +1.79933    +2.43410    +1.99634
O   +1.39960    +3.05702    +0.89021
C   +0.83027    +4.33903    +1.09317
O   +1.72118    +2.92595    +3.08941
H   +0.56039    +4.70275    +0.11026
H   -0.04732    +4.25998    +1.72753
H   +1.54965    +5.00158    +1.56397
H   +3.24917    +0.94657    +2.26418
H   +2.51959    +0.94459    +0.65896
H   +1.17295    +0.13109    +3.27525
H   +1.79401    -0.98054    +2.07731
H   -0.62240    +1.13236    +1.84763
H   -0.68764    -0.72189    +1.93122
H   -1.01396    -0.03246    -0.38960
H   +0.48175    +0.88929    -0.40001
H   +0.53079    -0.87130    -0.39001
H   -1.07358    +1.91906    +2.07641

* E =  +1.728 kcal/mol ; Conformer 016
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49956
C   +1.32325    +0.00000    +2.21221
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C    +2.05438    -1.33922    +2.15992
C    +2.52089    -1.73717    +0.79399
O    +3.18158    -0.75188    +0.18834
C    +3.64705    -1.04622    -1.11620
O    +2.34716    -2.81175    +0.28510
H    +4.17076    -0.16066    -1.45204
H    +4.31350    -1.90261    -1.09802
H    +2.81043    -1.26673    -1.77290
H    +2.94001    -1.28618    +2.79356
H    +1.43180    -2.14723    +2.53199
H    +1.96715    +0.77244    +1.79451
H    +1.16321    +0.25029    +3.26007
H    -0.54010    +1.15831    +1.83940
H    -0.71755    -0.69418    +1.93208
H    -0.99075    +0.22549    -0.38806
H    +0.69614    +0.73981    -0.39016
H    +0.28541    -0.97279    -0.40314
H    -0.89805    +1.99699    +2.07457

* E =   +1.796 kcal/mol ; Conformer 017
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49815
C    +1.33425    +0.00000    +2.18634
C    +2.08686    -1.31372    +1.98634
C    +3.40390    -1.34192    +2.69640
O    +4.18642    -0.32898    +2.32682
C    +5.45589    -0.28207    +2.95381
O    +3.74223    -2.16379    +3.50438
H    +5.95460    +0.58906    +2.54932
H    +5.34343    -0.19342    +4.02976
H    +6.02022    -1.18280    +2.73349
H    +1.50861    -2.15690    +2.35141
H    +2.27986    -1.46889    +0.92537
H    +1.94566    +0.81862    +1.80967
H    +1.19378    +0.17161    +3.25315
H    -0.54591    +1.16171    +1.84311
H    -0.71096    -0.69789    +1.93470
H    -0.99939    +0.16588    -0.39465
H    +0.65144    +0.77960    -0.39095
H    +0.34987    -0.95273    -0.40065
H    -0.90331    +1.99694    +2.06985

* E =   +1.807 kcal/mol ; Conformer 018
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49815
C    +1.33237    +0.00000    +2.18983
C    +2.08103    -1.31799    +2.00202
C    +3.40346    -1.33562    +2.70324
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O    +3.27200   -1.11873   +4.01100
C    +4.48003   -1.11624   +4.75094
O    +4.46811   -1.51855   +2.17807
H    +4.19820   -0.92695   +5.77852
H    +4.98024   -2.07549   +4.66179
H    +5.14488   -0.33916   +4.38719
H    +1.47922   -2.13530   +2.39921
H    +2.27641   -1.51833   +0.95381
H    +1.94185   +0.81680   +1.80121
H    +1.19961   +0.17923   +3.25471
H    -0.54835   +1.16060   +1.84291
H    -0.70950   -0.69956   +1.93505
H    -1.00040   +0.15876   -0.39493
H    +0.64578   +0.78441   -0.39063
H    +0.35842   -0.94943   -0.40053
H    -0.90776   +1.99489   +2.07030

* E =  +1.991 kcal/mol ; Conformer 019
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49850
C    +1.32477   +0.00000   +2.20742
C    +2.23661   +1.14111   +1.78063
C    +3.52643   +1.18779   +2.53865
O    +3.33395   +1.15064   +3.85634
C    +4.50959   +1.21635   +4.64361
O    +4.61889   +1.26358   +2.04473
H    +4.17972   +1.17454   +5.67351
H    +5.16423   +0.38070   +4.41697
H    +5.04318   +2.14165   +4.45012
H    +2.49777   +1.08040   +0.72960
H    +1.72324   +2.08977   +1.94330
H    +1.16285   +0.05774   +3.28146
H    +1.82998   -0.95286   +2.02190
H    -0.56781   +1.15602   +1.85210
H    -0.69916   -0.71154   +1.92900
H    -1.01352   -0.00974   -0.39180
H    +0.50239   +0.87504   -0.40645
H    +0.51336   -0.88142   -0.38963
H    -0.92891   +1.98632   +2.09072

* E =  +2.041 kcal/mol ; Conformer 020
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49863
C    +1.32015   +0.00000   +2.21821
C    +2.27918   +1.09274   +1.77179
C    +2.95783   +0.87725   +0.45284
O    +3.26827   -0.40104   +0.24163
C    +3.95258   -0.66452   -0.97028
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O    +3.23843   +1.74831   -0.32565
H    +4.13251   -1.73170   -0.98384
H    +3.34453   -0.36779   -1.81934
H    +4.88951   -0.11756   -1.00306
H    +1.78654   +2.06008   +1.72085
H    +3.08314   +1.18716   +2.50250
H    +1.13372   +0.12177   +3.28425
H    +1.80490   -0.97078   +2.09876
H    -0.56329   +1.15358   +1.85018
H    -0.70253   -0.70846   +1.92948
H    -1.01491   -0.00371   -0.38872
H    +0.50176   +0.87628   -0.40661
H    +0.51016   -0.88284   -0.38941
H    -0.92138   +1.98441   +2.10302

* E =  +7.834 kcal/mol ; Conformer 021
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49621
C    +1.34291   +0.00000   +2.16445
C    +1.25515   +0.10540   +3.67314
C    +0.71563   -1.15175   +4.30159
O    +0.45694   -1.13161   +5.61404
C    +0.63186   +0.03939   +6.37823
O    +0.53006   -2.16503   +3.69197
H    +0.43213   -0.24649   +7.40335
H    +1.64810   +0.41965   +6.30831
H    -0.07092   +0.81539   +6.08382
H    +2.24009   +0.29184   +4.10366
H    +0.63667   +0.95627   +3.95812
H    +1.87463   -0.91672   +1.90227
H    +1.93560   +0.83264   +1.78502
H    -0.53466   +1.17175   +1.84795
H    -0.69712   -0.70684   +1.93661
H    -1.00557   +0.10793   -0.39815
H    +0.61006   +0.81015   -0.39587
H    +0.40710   -0.93656   -0.38428
H    -0.85030   +2.02259   +2.08576

* E =  +8.178 kcal/mol ; Conformer 022
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49707
C    +1.34090   +0.00000   +2.16703
C    +1.23737   +0.12657   +3.67112
C    +2.58735   +0.09465   +4.33187
O    +2.63560   +0.25152   +5.66074
C    +1.46611   +0.47261   +6.41443
O    +3.60861   -0.06995   +3.73096
H    +1.78761   +0.52668   +7.44698
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H   +0.98683   +1.41048   +6.14335
H   +0.75667   -0.34462   +6.30729
H   +0.72428   +1.05030   +3.94017
H   +0.62928   -0.68086   +4.08324
H   +1.88459   -0.91440   +1.92088
H   +1.95284   +0.81311   +1.77844
H   -0.54968   +1.16094   +1.84795
H   -0.70643   -0.70313   +1.93442
H   -1.00630   +0.09521   -0.39958
H   +0.59935   +0.81964   -0.39113
H   +0.42351   -0.92768   -0.38824
H   -0.89188   +2.00376   +2.08469

* E =  +8.867 kcal/mol ; Conformer 023
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49890
C   +1.32404   +0.00000   +2.20756
C   +2.21639   +1.16024   +1.81842
C   +3.49746   +1.16257   +2.60541
O   +4.35364   +2.17148   +2.39979
C   +4.05423   +3.21440   +1.50147
O   +3.78742   +0.30925   +3.39209
H   +4.91973   +3.86504   +1.50741
H   +3.89766   +2.84373   +0.49110
H   +3.18319   +3.78127   +1.82199
H   +2.46846   +1.12637   +0.75799
H   +1.69547   +2.10641   +1.97100
H   +1.16872   +0.02296   +3.28391
H   +1.85203   -0.93565   +2.01034
H   -0.57037   +1.15532   +1.84827
H   -0.69940   -0.71206   +1.92742
H   -1.01295   -0.00921   -0.39331
H   +0.50201   +0.87541   -0.40757
H   +0.51300   -0.88190   -0.38880
H   -0.92672   +1.99139   +2.07891

* E =  +8.934 kcal/mol ; Conformer 024
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49843
C   +1.33559   +0.00000   +2.18707
C   +2.14320   -1.26654   +1.95341
C   +1.53004   -2.46813   +2.62105
O   +2.08967   -3.66268   +2.39157
C   +3.20076   -3.80127   +1.53667
O   +0.58688   -2.40459   +3.35442
H   +3.49035   -4.84288   +1.59741
H   +2.94356   -3.56588   +0.50629
H   +4.03598   -3.18249   +1.85577
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H    +2.26543    -1.46142    +0.88835
H    +3.15332    -1.14608    +2.34876
H    +1.92362    +0.84696    +1.83242
H    +1.19079    +0.12789    +3.25739
H    -0.52353    +1.17442    +1.83364
H    -0.71049    -0.68715    +1.94605
H    -0.99829    +0.17672    -0.39269
H    +0.65877    +0.77164    -0.39603
H    +0.33402    -0.95769    -0.40388
H    -0.84706    +2.02728    +2.04352


* E =  +8.961 kcal/mol ; Conformer 025
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49776
C    +1.31838    +0.00000    +2.22121
C    +2.26673    +1.09532    +1.76792
C    +3.07675    +0.70596    +0.55933
O    +3.78936    +1.66251    -0.04742
C    +3.75853    +2.99885    +0.39956
O    +3.13871    -0.41251    +0.13805
H    +4.49548    +3.52392    -0.19520
H    +2.78340    +3.45156    +0.23500
H    +4.02749    +3.08015    +1.44985
H    +1.72027    +2.01852    +1.57659
H    +2.97943    +1.33092    +2.55993
H    +1.12978    +0.11541    +3.28710
H    +1.81121    -0.96399    +2.08565
H    -0.55175    +1.15593    +1.84480
H    -0.70526    -0.70546    +1.92870
H    -1.01546    +0.02257    -0.38688
H    +0.52563    +0.86281    -0.40647
H    +0.49964    -0.88653    -0.38971
H    -0.88716    +2.00457    +2.08821


* E =  +9.084 kcal/mol ; Conformer 026
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49866
C    +1.33222    +0.00000    +2.19087
C    +2.07684    -1.31090    +2.01376
C    +3.39808    -1.30438    +2.73380
O    +4.15391    -2.40805    +2.65976
C    +3.73260    -3.53759    +1.93174
O    +3.79931    -0.36944    +3.36190
H    +4.52313    -4.26945    +2.04077
H    +2.80981    -3.95234    +2.33092
H    +3.60467    -3.31059    +0.87577
H    +1.47771    -2.14500    +2.38254
H    +2.25594    -1.51768    +0.95812
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H   +1.95188   +0.81134   +1.81205
H   +1.20689   +0.18953   +3.25471
H   -0.54744   +1.16325   +1.83939
H   -0.71580   -0.69419   +1.93427
H   -0.99889   +0.16599   -0.39598
H   +0.65094   +0.78066   -0.38969
H   +0.35068   -0.95188   -0.40309
H   -0.90747   +1.99685   +2.06144


* E =  +9.723 kcal/mol ; Conformer 027
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49774
C   +1.32041   +0.00000   +2.21664
C   +2.08905   -1.30635   +2.07394
C   +2.89757   -1.38064   +0.80507
O   +3.43382   -2.56311   +0.47718
C   +3.23282   -3.71003   +1.27048
O   +3.11123   -0.43763   +0.10101
H   +3.86530   -4.47761   +0.84222
H   +3.52766   -3.54409   +2.30379
H   +2.19827   -4.04404   +1.23350
H   +2.79508   -1.42013   +2.89913
H   +1.41582   -2.16022   +2.14165
H   +1.94381   +0.81156   +1.84676
H   +1.14261   +0.18006   +3.27551
H   -0.54681   +1.15716   +1.84668
H   -0.71630   -0.69596   +1.93177
H   -1.00101   +0.17604   -0.38730
H   +0.66980   +0.76004   -0.39287
H   +0.33978   -0.95621   -0.40133
H   -0.90595   +1.98860   +2.09318


* E =  +9.760 kcal/mol ; Conformer 028
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49671
C   +1.33916   +0.00000   +2.17030
C   +1.22058   +0.01763   +3.69175
C   +2.57854   +0.15089   +4.32151
O   +3.07277   +1.37975   +4.51875
C   +2.29156   +2.53402   +4.30322
O   +3.25551   -0.79620   +4.59899
H   +1.87196   +2.56414   +3.30051
H   +1.49118   +2.60950   +5.03576
H   +2.96576   +3.37198   +4.43014
H   +0.54663   +0.81284   +4.00094
H   +0.80889   -0.92557   +4.03679
H   +1.91197   -0.88114   +1.87317
H   +1.91324   +0.86077   +1.82109
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H   -0.51557   +1.17210   +1.85177
H   -0.70926   -0.69514   +1.94025
H   -1.00519   +0.10918   -0.39836
H   +0.60997   +0.81113   -0.39299
H   +0.40914   -0.93413   -0.38766
H   -0.78823   +2.03842   +2.09855


* E =  +9.972 kcal/mol ; Conformer 029
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49643
C   +1.34252   +0.00000   +2.16945
C   +1.27412   +0.37551   +3.63824
C   +1.30503   +1.86981   +3.84333
O   +1.00080   +2.33888   +5.05936
C   +0.59518   +1.48055   +6.09976
O   +1.62956   +2.64295   +2.99114
H   +0.52408   +2.10312   +6.98300
H   -0.37996   +1.04346   +5.89685
H   +1.32126   +0.69147   +6.28087
H   +0.38797   -0.05316   +4.10405
H   +2.12719   -0.03140   +4.18400
H   +1.78057   -0.99668   +2.07524
H   +2.01159   +0.69229   +1.66327
H   -0.61731   +1.13885   +1.84829
H   -0.69092   -0.71965   +1.93284
H   -1.00951   +0.06088   -0.39847
H   +0.56937   +0.84225   -0.38716
H   +0.45437   -0.91213   -0.39197
H   -1.08936   +1.90830   +2.07589


* E = +10.126 kcal/mol ; Conformer 030
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49670
C   +1.33852   +0.00000   +2.17933
C   +2.20043   -1.22455   +1.84123
C   +1.47834   -2.50384   +2.16021
O   +1.58064   -3.01953   +3.39084
C   +2.46724   -2.48233   +4.34576
O   +0.76716   -3.04859   +1.36503
H   +2.27849   -3.02868   +5.26153
H   +3.50317   -2.63404   +4.05116
H   +2.28507   -1.42523   +4.52080
H   +2.39336   -1.24703   +0.77324
H   +3.15701   -1.15352   +2.35193
H   +1.89887   +0.88544   +1.87858
H   +1.19749   +0.07248   +3.25742
H   -0.53478   +1.16572   +1.85987
H   -0.70999   -0.70151   +1.92579
```

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H    -0.99099    +0.21468    -0.39201
H    +0.68900    +0.74416    -0.39725
H    +0.29464    -0.97906    -0.37893
H    -0.87270    +2.00281    +2.09918


 *  E = +10.165 kcal/mol ; Conformer 031
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49719
C    +1.35221    +0.00000    +2.17666
C    +1.54473    +1.14563    +3.15464
C    +1.66972    +2.46012    +2.42794
O    +1.64386    +3.58391    +3.15061
C    +1.39296    +3.55404    +4.53660
O    +1.82692    +2.53538    +1.24353
H    +1.51815    +4.57329    +4.88018
H    +0.37525    +3.23208    +4.74566
H    +2.09767    +2.91390    +5.06211
H    +0.72210    +1.18866    +3.86677
H    +2.45351    +1.00398    +3.74202
H    +1.49569    -0.93741    +2.71288
H    +2.13322    +0.06681    +1.42201
H    -0.60264    +1.13111    +1.83062
H    -0.70416    -0.70305    +1.93554
H    -1.00722    +0.08477    -0.40055
H    +0.59665    +0.82885    -0.37320
H    +0.43165    -0.92561    -0.38589
H    -1.05098    +1.92570    +2.07831
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 *  E = +10.267 kcal/mol ; Conformer 032
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49760
C    +1.32616    +0.00000    +2.20216
C    +2.26442    +1.10225    +1.71108
C    +3.46677    +1.18996    +2.60774
O    +3.38800    +1.95171    +3.70637
C    +2.28234    +2.79484    +3.94334
O    +4.46605    +0.56184    +2.40961
H    +2.43071    +3.20033    +4.93651
H    +2.25190    +3.61327    +3.22763
H    +1.33961    +2.25361    +3.91726
H    +2.63633    +0.86503    +0.72016
H    +1.72743    +2.04672    +1.65371
H    +1.15644    +0.10208    +3.27456
H    +1.82377    -0.96310    +2.06872
H    -0.53877    +1.16164    +1.86151
H    -0.70453    -0.70284    +1.93348
H    -1.01295    +0.01900    -0.39248
H    +0.52921    +0.86012    -0.40466
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H   +0.48840   -0.89596   -0.38798
H   -0.84708   +2.00549   +2.14014


* E = +10.364 kcal/mol ; Conformer 033
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49683
C   +1.34756   +0.00000   +2.15691
C   +1.27225   +0.00340   +3.68469
C   +0.69168   -1.28472   +4.19814
O   +1.51439   -2.32061   +4.41367
C   +2.91468   -2.18372   +4.33921
O   -0.48294   -1.44155   +4.36914
H   +3.31460   -3.18120   +4.47369
H   +3.23679   -1.80079   +3.37410
H   +3.29147   -1.54267   +5.13309
H   +2.25386   +0.19757   +4.10723
H   +0.60342   +0.79512   +4.00862
H   +1.92325   -0.86298   +1.80820
H   +1.90521   +0.88063   +1.83599
H   -0.51434   +1.17430   +1.84560
H   -0.71103   -0.68587   +1.94757
H   -1.00554   +0.11610   -0.39536
H   +0.61372   +0.80740   -0.39616
H   +0.39966   -0.93765   -0.39022
H   -0.79979   +2.04131   +2.06481


* E = +10.487 kcal/mol ; Conformer 034
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49714
C   +1.34181   +0.00000   +2.16636
C   +1.23875   +0.12901   +3.68315
C   +2.60789   +0.14617   +4.30465
O   +3.16447   -1.01530   +4.67517
C   +2.45508   -2.23020   +4.60826
O   +3.24036   +1.15342   +4.43319
H   +3.16969   -3.00236   +4.86546
H   +1.63823   -2.25201   +5.32618
H   +2.07178   -2.42290   +3.60898
H   +0.77642   +1.07957   +3.93030
H   +0.61311   -0.66376   +4.08583
H   +1.87855   -0.91620   +1.89969
H   +1.94561   +0.82298   +1.78460
H   -0.54809   +1.16496   +1.84660
H   -0.70411   -0.70297   +1.93761
H   -1.00697   +0.09730   -0.39719
H   +0.59835   +0.82028   -0.39128
H   +0.42061   -0.92773   -0.39172
H   -0.89371   +2.00633   +2.06701
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* E = +10.497 kcal/mol ; Conformer 035
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49916
C   +1.34904   +0.00000   +2.16988
C   +2.01995   +1.36359   +2.16889
C   +1.54546   +2.22007   +3.31657
O   +1.87656   +3.51649   +3.30567
C   +2.57185   +4.08874   +2.22275
O   +0.93044   +1.78880   +4.24694
H   +2.79519   +5.10540   +2.52153
H   +3.50403   +3.56735   +2.01816
H   +1.95805   +4.11138   +1.32503
H   +3.10171   +1.26492   +2.27267
H   +1.85539   +1.87866   +1.22361
H   +1.25885   −0.33325   +3.19928
H   +1.99613   −0.71073   +1.65035
H   −0.57884   +1.16335   +1.81244
H   −0.70358   −0.70403   +1.93152
H   −1.00277   +0.13074   −0.39887
H   +0.62235   +0.79820   −0.40268
H   +0.39068   −0.94251   −0.38705
H   −0.96293   +2.00776   +1.92207

* E = +10.713 kcal/mol ; Conformer 036
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49801
C   +1.33471   +0.00000   +2.18500
C   +2.09089   −1.31732   +1.98649
C   +3.43927   −1.25020   +2.64961
O   +3.55123   −1.63222   +3.92833
C   +2.47275   −2.21273   +4.62441
O   +4.40454   −0.81724   +2.09059
H   +2.81043   −2.32658   +5.64709
H   +1.59122   −1.57638   +4.61271
H   +2.22490   −3.19295   +4.22331
H   +1.49334   −2.15113   +2.34686
H   +2.28383   −1.47223   +0.92995
H   +1.95119   +0.81015   +1.79710
H   +1.19829   +0.19267   +3.24933
H   −0.54661   +1.15940   +1.84653
H   −0.70992   −0.69927   +1.93492
H   −1.00001   +0.16399   −0.39356
H   +0.64997   +0.78057   −0.39061
H   +0.35233   −0.95146   −0.40103
H   −0.90767   +1.99151   +2.08128

* E = +10.746 kcal/mol ; Conformer 037
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C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49822
C    +1.33287    +0.00000    +2.18802
C    +2.08334    -1.32259    +2.00255
C    +3.37105    -1.30505    +2.77951
O    +4.47909    -0.84459    +2.18436
C    +4.49848    -0.50714    +0.81671
O    +3.42885    -1.63761    +3.92739
H    +5.47515    -0.07621    +0.63424
H    +4.37887    -1.38851    +0.19054
H    +3.73631    +0.22723    +0.56763
H    +1.49058    -2.13320    +2.41529
H    +2.24454    -1.52491    +0.94717
H    +1.93581    +0.82756    +1.81058
H    +1.20118    +0.16945    +3.25507
H    -0.54629    +1.16216    +1.84169
H    -0.70806    -0.69963    +1.93602
H    -1.00042    +0.15850    -0.39469
H    +0.64320    +0.78661    -0.39163
H    +0.35661    -0.94984    -0.40180
H    -0.90257    +1.99875    +2.06336

* E = +11.138 kcal/mol ; Conformer 038
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49839
C    +1.32581    +0.00000    +2.20505
C    +2.22396    +1.17230    +1.81518
C    +3.47582    +1.16500    +2.64832
O    +4.55222    +0.50881    +2.19370
C    +4.57868    -0.06986    +0.90992
O    +3.53027    +1.68115    +3.72617
H    +3.75566    -0.76466    +0.75986
H    +4.56440    +0.69066    +0.13235
H    +5.51325    -0.61416    +0.85202
H    +2.44344    +1.15481    +0.75167
H    +1.71083    +2.10286    +2.03929
H    +1.16570    +0.03495    +3.28110
H    +1.83869    -0.94626    +2.00356
H    -0.57381    +1.15566    +1.85145
H    -0.69613    -0.71410    +1.92905
H    -1.01374    -0.00327    -0.39121
H    +0.50524    +0.87335    -0.40713
H    +0.50562    -0.88545    -0.39141
H    -0.94405    +1.98113    +2.08226

* E = +11.165 kcal/mol ; Conformer 039
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49747
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C    +1.35311    +0.00000    +2.14952
C    +1.32197    -0.28651    +3.65035
C    +0.34926    +0.59500    +4.38935
O    +0.75248    +1.79798    +4.81329
C    +2.09482    +2.20938    +4.70022
O    -0.78525    +0.26528    +4.58167
H    +2.11365    +3.24278    +5.02366
H    +2.74271    +1.62469    +5.34974
H    +2.45301    +2.15469    +3.67588
H    +0.96816    -1.30038    +3.81017
H    +2.32510    -0.21359    +4.06271
H    +1.98355    -0.76060    +1.68249
H    +1.84491    +0.95331    +1.94616
H    -0.52615    +1.17057    +1.82452
H    -0.70802    -0.68812    +1.95071
H    -1.00455    +0.12188    -0.39610
H    +0.61632    +0.80679    -0.39376
H    +0.39842    -0.93753    -0.39138
H    -0.80983    +2.04875    +2.00154

* E = +11.267 kcal/mol ; Conformer 040
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49901
C    +1.33079    +0.00000    +2.20375
C    +1.85662    -1.39868    +2.55004
C    +1.94764    -2.29218    +1.34523
O    +3.04172    -2.23387    +0.57562
C    +4.18586    -1.51214    +0.97196
O    +1.05238    -3.01695    +1.01730
H    +4.87480    -1.57316    +0.13867
H    +3.96138    -0.46755    +1.16959
H    +4.64989    -1.96126    +1.84717
H    +2.81207    -1.31397    +3.06225
H    +1.15736    -1.88345    +3.22404
H    +2.05735    +0.54327    +1.59925
H    +1.24851    +0.54536    +3.14410
H    -0.54158    +1.15119    +1.83486
H    -0.70960    -0.69987    +1.93362
H    -1.00552    +0.14180    -0.38839
H    +0.62665    +0.80067    -0.38948
H    +0.36998    -0.94412    -0.39840
H    -0.89554    +1.99268    +2.08357

* E = +12.221 kcal/mol ; Conformer 041
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49679
C    +1.32384    +0.00000    +2.20984
C    +2.25228    +1.15502    +1.79897
```

```
C    +3.21625    +0.76861    +0.71174
O    +4.25773    -0.00756    +1.04889
C    +4.61254    -0.22430    +2.39557
O    +3.08388    +1.08056    -0.43578
H    +5.43102    -0.93322    +2.37310
H    +4.95611    +0.69615    +2.86283
H    +3.79552    -0.64570    +2.97535
H    +1.66831    +1.98838    +1.42099
H    +2.80367    +1.51321    +2.66484
H    +1.14220    +0.05457    +3.28185
H    +1.81874    -0.95989    +2.03535
H    -0.55425    +1.15646    +1.85906
H    -0.69985    -0.70727    +1.93425
H    -1.01387    +0.06000    -0.38698
H    +0.57401    +0.82771    -0.40812
H    +0.44819    -0.91697    -0.38774
H    -0.89989    +1.98842    +2.12124
```

S.2.6 $(\mathbf{TS}_\delta)^\ddagger$

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* E =  +0.000 kcal/mol ; Conformer 001
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49535
C    +1.40110    +0.00000    +2.07976
C    +1.41393    +0.00536    +3.59306
C    +0.93933    +1.30088    +4.17712
O    +0.71710    +1.19859    +5.48536
C    +0.30435    +2.39231    +6.12702
O    +0.78946    +2.32685    +3.56938
H    +0.17077    +2.13697    +7.17014
H    +1.06037    +3.16332    +6.01590
H    -0.62675    +2.74999    +5.69880
H    +0.80804    -0.79940    +4.00685
H    +2.42196    -0.15526    +3.97609
H    +1.93845    -0.87846    +1.72499
H    +1.94056    +0.87426    +1.71799
H    -0.53539    +0.88188    +1.85589
H    -0.55077    -0.86868    +1.86116
H    +0.61683    -1.16783    -0.37345
H    -0.96726    -0.09648    -0.47954
H    +0.62707    +0.75028    -0.47027
H    +1.02017    -1.95797    -0.57060

* E =  +0.320 kcal/mol ; Conformer 002
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49582
C    +1.40950    +0.00000    +2.07384
C    +1.42421    -0.00003    +3.58832
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C    +0.95122    +1.29497    +4.17514
O    +0.70334    +1.18346    +5.47775
C    +0.29172    +2.37625    +6.12228
O    +0.82488    +2.32736    +3.57331
H    +0.13615    +2.11337    +7.16045
H    +1.05803    +3.13974    +6.03173
H    -0.62737    +2.74754    +5.68003
H    +0.81912    -0.80603    +4.00038
H    +2.43366    -0.16026    +3.96824
H    +1.94852    -0.87682    +1.71717
H    +1.94704    +0.87585    +1.71466
H    -0.53016    +0.87809    +1.86164
H    -0.53616    -0.87653    +1.86332
H    -1.31661    -0.02250    -0.38978
H    +0.35731    +0.90930    -0.47101
H    +0.38705    -0.89522    -0.47573
H    -2.19378    -0.04084    -0.60947

* E =   +0.332 kcal/mol ; Conformer 003
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49783
C    +1.38510    +0.00000    +2.12515
C    +2.26487    -1.16214    +1.71067
C    +1.73461    -2.49117    +2.15169
O    +2.38772    -3.49613    +1.57519
C    +1.96076    -4.79309    +1.95060
O    +0.84743    -2.65951    +2.94552
H    +2.58667    -5.48231    +1.39885
H    +2.08172    -4.93825    +3.01965
H    +0.91615    -4.93568    +1.69233
H    +2.41901    -1.20024    +0.63431
H    +3.25855    -1.06207    +2.14822
H    +1.89906    +0.92442    +1.86080
H    +1.27939    -0.00675    +3.20804
H    -0.53451    +0.88548    +1.85067
H    -0.56574    -0.85439    +1.86755
H    +0.29129    -1.26843    -0.41032
H    -0.96964    +0.13020    -0.46715
H    +0.77368    +0.58992    -0.48320
H    +0.45237    -2.13402    -0.65117

* E =   +0.452 kcal/mol ; Conformer 004
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49606
C    +1.40714    +0.00000    +2.07658
C    +1.39827    -0.00002    +3.58897
C    +2.77513    -0.00001    +4.17562
O    +2.74095    +0.00018    +5.50680
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C    +4.00496    +0.00017    +6.14642
O    +3.79984    -0.00016    +3.54910
H    +3.79942    +0.00042    +7.20895
H    +4.57113    -0.88281    +5.86684
H    +4.57133    +0.88289    +5.86647
H    +0.87037    +0.86813    +3.98402
H    +0.87041    -0.86823    +3.98399
H    +1.95769    -0.86881    +1.71953
H    +1.95767    +0.86883    +1.71955
H    -0.54111    +0.87371    +1.86204
H    -0.54111    -0.87371    +1.86204
H    -1.31845    +0.00003    -0.38834
H    +0.37324    +0.90178    -0.47334
H    +0.37320    -0.90180    -0.47334
H    -2.19609    +0.00007    -0.60324

* E =   +0.453 kcal/mol ; Conformer 005
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49587
C    +1.40027    +0.00000    +2.08267
C    +1.41400    -0.09078    +3.59345
C    +0.88520    +1.14120    +4.26234
O    +0.66966    +0.94009    +5.56079
C    +0.20833    +2.06916    +6.28144
O    +0.69085    +2.19843    +3.72602
H    +0.08781    +1.73855    +7.30484
H    +0.93087    +2.87720    +6.22320
H    -0.73788    +2.41549    +5.87770
H    +0.84315    -0.94584    +3.95294
H    +2.42847    -0.23298    +3.96675
H    +1.96165    -0.84244    +1.67877
H    +1.91699    +0.90680    +1.77277
H    -0.54559    +0.86786    +1.86398
H    -0.54095    -0.88219    +1.85538
H    +0.63380    +1.15526    -0.38528
H    +0.61550    -0.75886    -0.47300
H    -0.96656    +0.10949    -0.47805
H    +1.05104    +1.92885    -0.60992

* E =   +0.478 kcal/mol ; Conformer 006
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49589
C    +1.39840    +0.00000    +2.08363
C    +1.38502    +0.01531    +3.59509
C    +2.75777    -0.03602    +4.18875
O    +2.72226    +0.06869    +5.51612
C    +3.98174    +0.01815    +6.16241
O    +3.78044    -0.16103    +3.57166
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H    +3.77622    +0.11713    +7.22035
H    +4.47633    -0.92586    +5.95588
H    +4.61665    +0.82883    +5.81886
H    +0.88609    +0.90322    +3.98257
H    +0.82644    -0.83231    +3.99441
H    +1.94702    -0.87502    +1.73816
H    +1.95185    +0.86324    +1.71704
H    -0.55580    +0.86629    +1.85933
H    -0.54654    -0.87655    +1.85870
H    +0.57207    +1.18921    -0.37069
H    +0.65478    -0.72467    -0.47259
H    -0.97038    +0.06278    -0.47877
H    +0.94140    +1.99532    -0.56764


* E =  +0.491 kcal/mol ; Conformer 007
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49758
C    +1.37611    +0.00000    +2.14462
C    +2.20911    +1.23388    +1.85006
C    +2.98293    +1.15246    +0.56927
O    +3.48027    +2.33646    +0.22598
C    +4.23647    +2.35355    -0.97115
O    +3.17653    +0.15301    -0.07014
H    +4.56728    +3.37616    -1.09800
H    +5.08642    +1.68273    -0.89386
H    +3.61895    +2.04573    -1.80931
H    +1.60427    +2.13923    +1.82397
H    +2.94998    +1.39342    +2.63406
H    +1.24666    -0.08178    +3.22208
H    +1.93196    -0.87964    +1.82311
H    -0.57491    +0.85409    +1.86247
H    -0.53975    -0.88546    +1.84428
H    +0.38788    +1.24230    -0.41967
H    +0.73648    -0.63688    -0.47605
H    -0.97992    -0.05615    -0.46110
H    +0.60809    +2.08770    -0.68301


* E =  +0.656 kcal/mol ; Conformer 008
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49817
C    +1.38244    +0.00000    +2.12604
C    +2.20075    -1.22242    +1.77237
C    +3.50880    -1.26237    +2.49765
O    +4.21688    -2.34303    +2.17510
C    +5.47263    -2.46022    +2.81932
O    +3.89936    -0.43753    +3.27926
H    +5.90996    -3.37916    +2.45109
H    +6.10456    -1.61185    +2.57561
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H   +5.34396   -2.50306   +3.89640
H   +1.66288   -2.14227   +2.00448
H   +2.41449   -1.27693   +0.70583
H   +1.92511   +0.89421   +1.82066
H   +1.29289   +0.06343   +3.20839
H   -0.53879   +0.88365   +1.84884
H   -0.57358   -0.85539   +1.86164
H   +0.30607   -1.26414   -0.42398
H   -0.96937   +0.12564   -0.46900
H   +0.77019   +0.59985   -0.47565
H   +0.47322   -2.11933   -0.68527

* E =  +0.683 kcal/mol ; Conformer 009
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49702
C   +1.38724   +0.00000   +2.12181
C   +2.20042   -1.24582   +1.83479
C   +1.63695   -2.47308   +2.48307
O   +2.18495   -3.58389   +1.99546
C   +1.74309   -4.79122   +2.59067
O   +0.80958   -2.48404   +3.35473
H   +2.28114   -5.58391   +2.08739
H   +1.96496   -4.79326   +3.65328
H   +0.67263   -4.91032   +2.45591
H   +2.31200   -1.43893   +0.77018
H   +3.21563   -1.13489   +2.21712
H   +1.94178   +0.86669   +1.76403
H   +1.28626   +0.10431   +3.19989
H   -0.54291   +0.87553   +1.85181
H   -0.55650   -0.86403   +1.86893
H   +0.65569   +1.14440   -0.37522
H   +0.58659   -0.76885   -0.49147
H   -0.96679   +0.13560   -0.47120
H   +1.08445   +1.92059   -0.57943

* E =  +0.910 kcal/mol ; Conformer 010
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49775
C   +1.39850   +0.00000   +2.10899
C   +2.21553   -1.23263   +1.78037
C   +1.67167   -2.47682   +2.41328
O   +2.19250   -3.57467   +1.86995
C   +1.76714   -4.79766   +2.44523
O   +0.88071   -2.50966   +3.31736
H   +2.27800   -5.57722   +1.89530
H   +2.03315   -4.83443   +3.49702
H   +0.69117   -4.90593   +2.35179
H   +2.30204   -1.39858   +0.70869
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H   +3.23721   -1.12391   +2.14580
H   +1.94335   +0.87904   +1.76622
H   +1.30669   +0.07932   +3.19056
H   -0.52635   +0.88430   +1.85574
H   -0.55082   -0.86017   +1.87488
H   -1.30637   +0.13930   -0.38020
H   +0.45957   +0.86237   -0.47284
H   +0.26630   -0.93000   -0.49042
H   -2.18186   +0.24040   -0.59617

* E =  +0.928 kcal/mol ; Conformer 011
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49778
C   +1.39585   +0.00000   +2.11040
C   +2.19486   -1.23682   +1.76466
C   +3.52291   -1.27564   +2.45333
O   +4.21514   -2.36430   +2.12287
C   +5.48738   -2.48343   +2.73432
O   +3.93869   -0.44460   +3.21440
H   +5.90879   -3.40881   +2.36378
H   +6.11759   -1.64162   +2.46499
H   +5.38727   -2.51473   +3.81477
H   +1.65590   -2.14490   +2.03811
H   +2.37835   -1.31571   +0.69376
H   +1.94316   +0.88402   +1.78614
H   +1.31626   +0.07835   +3.19306
H   -0.53118   +0.88133   +1.85589
H   -0.55560   -0.86429   +1.86385
H   -1.30646   +0.15199   -0.37861
H   +0.46742   +0.85969   -0.46948
H   +0.26078   -0.93222   -0.48883
H   -2.18193   +0.26253   -0.58646

* E =  +1.008 kcal/mol ; Conformer 012
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49553
C   +1.39951   +0.00000   +2.08280
C   +1.40338   -0.00570   +3.60078
C   +0.75467   +1.19127   +4.22772
O   +1.05574   +2.32054   +3.58675
C   +0.50926   +3.50035   +4.14860
O   +0.06187   +1.16843   +5.20872
H   +0.84185   +4.31260   +3.51538
H   -0.57482   +3.44581   +4.16372
H   +0.86644   +3.63635   +5.16459
H   +0.89710   -0.87998   +4.00016
H   +2.42887   -0.03345   +3.97001
H   +1.93791   -0.87837   +1.72911
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H    +1.94368    +0.87198    +1.72380
H    -0.54127    +0.88105    +1.85508
H    -0.55472    -0.86427    +1.86390
H    +0.61093    -1.16964    -0.37336
H    -0.96762    -0.09220    -0.47944
H    +0.63161    +0.74582    -0.47150
H    +1.01165    -1.96028    -0.57376


* E =   +1.076 kcal/mol ; Conformer 013
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49748
C    +1.38347    +0.00000    +2.12674
C    +2.18773    -1.24063    +1.80480
C    +3.48160    -1.29758    +2.55562
O    +4.22479    -2.33429    +2.17223
C    +5.46343    -2.47412    +2.84501
O    +3.83012    -0.52543    +3.40686
H    +5.93461    -3.35057    +2.41947
H    +6.08045    -1.59475    +2.68919
H    +5.30350    -2.60565    +3.91065
H    +1.63045    -2.14562    +2.05297
H    +2.42137    -1.31953    +0.74461
H    +1.93459    +0.88129    +1.80138
H    +1.29259    +0.08485    +3.20728
H    -0.54945    +0.87077    +1.85346
H    -0.55892    -0.87065    +1.85686
H    +0.67405    +1.13477    -0.37748
H    +0.57565    -0.77892    -0.48802
H    -0.96421    +0.15029    -0.47189
H    +1.11327    +1.90073    -0.59081


* E =   +1.109 kcal/mol ; Conformer 014
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49571
C    +1.39871    +0.00000    +2.08493
C    +1.39995    -0.03682    +3.60299
C    +0.73168    +1.14019    +4.24727
O    +1.04829    +2.28603    +3.64678
C    +0.47865    +3.44983    +4.21844
O    +0.01003    +1.08730    +5.20629
H    +0.82558    +4.27761    +3.61377
H    -0.60504    +3.38957    +4.19905
H    +0.80425    +3.56423    +5.24766
H    +0.90315    -0.92482    +3.98366
H    +2.42506    -0.05716    +3.97336
H    +1.94676    -0.86720    +1.71685
H    +1.93467    +0.88317    +1.74255
H    -0.55024    +0.86986    +1.85854
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H   -0.54713   -0.87490   +1.86071
H   +0.60126   +1.17451   -0.37647
H   +0.63668   -0.74084   -0.47290
H   -0.96884   +0.08407   -0.47849
H   +0.99251   +1.96694   -0.58352


* E =  +1.150 kcal/mol ; Conformer 015
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49743
C   +1.39388   +0.00000   +2.11908
C   +2.24047   +1.19224   +1.71383
C   +2.88990   +1.02155   +0.37403
O   +3.10549   +2.18901   -0.22746
C   +3.77525   +2.11458   -1.47401
O   +3.22106   -0.02930   -0.10604
H   +3.87257   +3.13555   -1.81937
H   +4.75188   +1.65665   -1.35258
H   +3.19719   +1.52548   -2.17905
H   +1.67155   +2.11964   +1.71830
H   +3.05965   +1.33068   +2.42048
H   +1.28824   -0.00762   +3.20257
H   +1.92398   -0.90940   +1.84120
H   -0.55200   +0.86761   +1.86136
H   -0.53392   -0.87919   +1.85782
H   -1.30765   -0.16368   -0.37603
H   +0.24712   +0.93977   -0.48363
H   +0.48584   -0.84685   -0.47159
H   -2.18154   -0.28383   -0.58252


* E =  +1.265 kcal/mol ; Conformer 016
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49593
C   +1.40829   +0.00000   +2.07582
C   +1.41787   -0.01798   +3.59469
C   +0.76711   +1.17048   +4.23570
O   +1.04939   +2.30519   +3.59645
C   +0.49789   +3.47724   +4.17008
O   +0.08881   +1.13571   +5.22627
H   +0.81495   +4.29539   +3.53651
H   -0.58529   +3.41166   +4.19734
H   +0.86579   +3.61222   +5.18235
H   +0.91708   -0.89781   +3.98877
H   +2.44528   -0.04440   +3.95900
H   +1.94976   -0.87402   +1.71566
H   +1.94801   +0.87610   +1.72158
H   -0.53482   +0.87792   +1.86041
H   -0.54062   -0.87188   +1.86595
H   -1.31632   +0.00075   -0.39130
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H    +0.37483    +0.90171    -0.47234
H    +0.37203    -0.90221    -0.47394
H    -2.19310    +0.00017    -0.61257


* E =   +1.333 kcal/mol ; Conformer 017
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49587
C    +1.39867    +0.00000    +2.08390
C    +1.37895    -0.00398    +3.60320
C    +2.74108    -0.00935    +4.22347
O    +3.51190    -0.97446    +3.72318
C    +4.81526    -1.05524    +4.27177
O    +3.11865    +0.74378    +5.07963
H    +5.30205    -1.87585    +3.76091
H    +5.35395    -0.12768    +4.10557
H    +4.76561    -1.24478    +5.33949
H    +0.85655    +0.86358    +3.99507
H    +0.85579    -0.89279    +3.95883
H    +1.94833    -0.87013    +1.72904
H    +1.93765    +0.87784    +1.72699
H    -0.55479    +0.86540    +1.86146
H    -0.54321    -0.87822    +1.85941
H    +0.59824    +1.17605    -0.37324
H    +0.63842    -0.73928    -0.47253
H    -0.96897    +0.08292    -0.47841
H    +0.98864    +1.97123    -0.57406


* E =   +1.336 kcal/mol ; Conformer 018
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49588
C    +1.39833    +0.00000    +2.08464
C    +1.37772    +0.01433    +3.60448
C    +2.74307    +0.02810    +4.21705
O    +3.49538    -0.97806    +3.77392
C    +4.80338    -1.04219    +4.31335
O    +3.13918    +0.83127    +5.01786
H    +5.27254    -1.90171    +3.85252
H    +5.35355    -0.13572    +4.08122
H    +4.76280    -1.16067    +5.39167
H    +0.85084    +0.88441    +3.98467
H    +0.86131    -0.87424    +3.96914
H    +1.94301    -0.87617    +1.73827
H    +1.94250    +0.87230    +1.72030
H    -0.54676    +0.87570    +1.85924
H    -0.55133    -0.86793    +1.86150
H    +0.59851    -1.17617    -0.37389
H    -0.96917    -0.08258    -0.47808
H    +0.63781    +0.73969    -0.47276
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H    +0.98844    -1.97113    -0.57500


* E =   +1.363 kcal/mol ; Conformer 019
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49602
C    +1.40751    +0.00000    +2.07636
C    +1.39315    +0.00684    +3.59770
C    +2.76407    +0.01430    +4.19738
O    +3.49569    -1.01543    +3.77244
C    +4.80919    -1.08465    +4.29799
O    +3.18258    +0.83226    +4.97110
H    +5.25972    -1.96402    +3.85639
H    +5.37015    -0.19371    +4.03377
H    +4.78005    -1.17205    +5.37960
H    +0.87198    +0.87811    +3.98242
H    +0.87551    -0.88168    +3.95997
H    +1.95316    -0.87403    +1.72595
H    +1.94837    +0.87454    +1.71404
H    -0.54053    +0.87279    +1.86368
H    -0.53683    -0.87543    +1.86373
H    -1.31702    -0.00956    -0.38775
H    +0.36599    +0.90458    -0.47372
H    +0.37916    -0.89933    -0.47337
H    -2.19484    -0.01672    -0.60435


* E =   +1.417 kcal/mol ; Conformer 020
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49759
C    +1.38807    +0.00000    +2.12240
C    +2.27829    -1.13939    +1.64063
C    +1.62290    -2.47442    +1.80502
O    +1.34668    -2.73539    +3.08229
C    +0.70815    -3.97614    +3.32517
O    +1.34784    -3.23197    +0.91334
H    +0.55760    -4.02826    +4.39562
H    -0.24229    -4.02224    +2.80256
H    +1.33343    -4.79633    +2.98664
H    +2.52812    -1.03193    +0.59021
H    +3.20643    -1.14046    +2.20916
H    +1.88806    +0.93982    +1.89310
H    +1.29170    -0.05756    +3.20448
H    -0.55099    +0.86352    +1.86742
H    -0.55139    -0.87790    +1.85196
H    +0.80180    +1.05282    -0.38386
H    +0.48342    -0.84584    -0.47673
H    -0.94207    +0.25459    -0.47120
H    +1.33336    +1.75479    -0.60137
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* E =  +1.532 kcal/mol ; Conformer 021
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49746
C   +1.39805    +0.00000    +2.10877
C   +2.25998    +1.17204    +1.65485
C   +1.58244    +2.48697    +1.88181
O   +1.32667    +2.69470    +3.17271
C   +0.66619    +3.91123    +3.47387
O   +1.27578    +3.27076    +1.02394
H   +0.53546    +3.92009    +4.54813
H   +1.26697    +4.75707    +3.15474
H   -0.29499    +3.95507    +2.97117
H   +3.19959    +1.17002    +2.20428
H   +2.48574    +1.11036    +0.59523
H   +1.31080    +0.02059    +3.19357
H   +1.91252    -0.92370    +1.84648
H   -0.54878    +0.87068    +1.85978
H   -0.53628    -0.87375    +1.86673
H   -1.31003    -0.14444    -0.37473
H   +0.26594    +0.93612    -0.47843
H   +0.46045    -0.86216    -0.47213
H   -2.18582    -0.25225    -0.57860

* E =  +1.656 kcal/mol ; Conformer 022
C   +0.00000    +0.00000    +0.00000
C   +0.00000    +0.00000    +1.49802
C   +1.38445    +0.00000    +2.12259
C   +2.20113    -1.23220    +1.76118
C   +3.52522    -1.27095    +2.45525
O   +4.24524    -0.17602    +2.20798
C   +5.51925    -0.13581    +2.82496
O   +3.92288    -2.16286    +3.15479
H   +5.96408    +0.80487    +2.52713
H   +5.41937    -0.18674    +3.90468
H   +6.12859    -0.96963    +2.49047
H   +1.67361    -2.14502    +2.02171
H   +2.38919    -1.25358    +0.68844
H   +1.92826    +0.89085    +1.81150
H   +1.28356    +0.05820    +3.20589
H   -0.53690    +0.88423    +1.85043
H   -0.57168    -0.85542    +1.86320
H   +0.29589    -1.26596    -0.42533
H   -0.96923    +0.13255    -0.46714
H   +0.77381    +0.59476    -0.47607
H   +0.45702    -2.12162    -0.68804

* E =  +1.710 kcal/mol ; Conformer 023
C   +0.00000    +0.00000    +0.00000
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C    +0.00000    +0.00000    +1.49805
C    +1.38311    +0.00000    +2.12530
C    +2.21405    -1.21708    +1.74142
C    +3.53194    -1.24433    +2.44854
O    +3.38179    -1.35447    +3.76905
C    +4.58423    -1.37920    +4.51646
O    +4.60978    -1.16983    +1.92339
H    +4.28796    -1.47357    +5.55315
H    +5.19926    -2.22192    +4.21648
H    +5.14614    -0.46344    +4.36118
H    +1.66847    -2.12520    +1.99745
H    +2.42190    -1.23814    +0.67707
H    +1.91405    +0.90443    +1.82510
H    +1.28754    +0.03490    +3.20851
H    -0.53899    +0.88230    +1.85197
H    -0.56889    -0.85775    +1.86281
H    +0.29038    -1.26900    -0.41894
H    -0.96845    +0.13666    -0.46746
H    +0.77754    +0.58870    -0.47717
H    +0.44625    -2.12831    -0.67201

*  E  =   +1.765 kcal/mol ; Conformer 024
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49833
C    +1.39086    +0.00000    +2.12614
C    +2.20433    -1.25389    +1.84500
C    +2.69156    -1.39746    +0.43574
O    +3.22790    -0.26848    -0.02571
C    +3.72547    -0.33191    -1.34989
O    +2.64801    -2.40756    -0.21399
H    +4.13047    +0.64894    -1.56275
H    +4.49720    -1.09091    -1.42989
H    +2.92424    -0.57293    -2.04219
H    +3.09378    -1.25461    +2.47566
H    +1.64280    -2.15418    +2.07871
H    +1.94875    +0.87172    +1.78847
H    +1.27997    +0.09518    +3.20548
H    -0.52993    +0.88350    +1.85481
H    -0.55758    -0.86274    +1.86396
H    -1.29628    +0.21233    -0.37384
H    +0.50564    +0.83907    -0.46664
H    +0.21529    -0.94314    -0.48972
H    -2.16639    +0.37205    -0.57934
21
*  E  =   +1.806 kcal/mol ; Conformer 025
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49750
C    +1.39746    +0.00000    +2.10768
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C   +2.19597   -1.24502   +1.75371
C   +3.53856   -1.29100   +2.41187
O   +4.24545   -0.18645   +2.17385
C   +5.53679   -0.15543   +2.75493
O   +3.95958   -2.20044   +3.07420
H   +5.96773   +0.79561   +2.47013
H   +5.46795   -0.23609   +3.83520
H   +6.14035   -0.97630   +2.38041
H   +1.66739   -2.14802   +2.04550
H   +2.35846   -1.28641   +0.67670
H   +1.94480   +0.88167   +1.77919
H   +1.30653   +0.07241   +3.19148
H   -0.52864   +0.88273   +1.85659
H   -0.55502   -0.86340   +1.86521
H   -1.30330   +0.17446   -0.37814
H   +0.48158   +0.85180   -0.46950
H   +0.24422   -0.93646   -0.48888
H   -2.17609   +0.30202   -0.58713

* E =  +1.869 kcal/mol ; Conformer 026
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49812
C   +1.37571   +0.00000   +2.14873
C   +2.22161   -1.22979   +1.84751
C   +2.80866   -1.27338   +0.46956
O   +3.37467   -0.11698   +0.13734
C   +3.92579   -0.05684   -1.16521
O   +2.79966   -2.22865   -0.26063
H   +4.35689   +0.93119   -1.25954
H   +4.68406   -0.82275   -1.29327
H   +3.14711   -0.20245   -1.90814
H   +3.06491   -1.26060   +2.53771
H   +1.65829   -2.14884   +1.98443
H   +1.92441   +0.89086   +1.84806
H   +1.24266   +0.06076   +3.22742
H   -0.55088   +0.86977   +1.85475
H   -0.55933   -0.87269   +1.85114
H   +0.73562   +1.09737   -0.39347
H   +0.51242   -0.82031   -0.49037
H   -0.95696   +0.21138   -0.46330
H   +1.20615   +1.83489   -0.62534

* E =  +1.876 kcal/mol ; Conformer 027
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49746
C   +1.39535   +0.00000   +2.11233
C   +2.19840   -1.24323   +1.75973
C   +3.54045   -1.27781   +2.42111
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O    +3.44107    -1.20513    +3.74821
C    +4.67008    -1.23662    +4.45154
O    +4.59567    -1.36304    +1.85350
H    +4.41353    -1.16966    +5.50083
H    +5.20042    -2.16114    +4.24569
H    +5.29658    -0.40062    +4.15679
H    +1.64822    -2.13026    +2.07609
H    +2.37183    -1.31766    +0.69128
H    +1.93695    +0.88603    +1.77961
H    +1.30948    +0.06997    +3.19486
H    -0.53115    +0.88122    +1.85647
H    -0.55281    -0.86512    +1.86530
H    -1.30804    +0.15137    -0.37706
H    +0.46650    +0.85987    -0.46981
H    +0.26147    -0.93179    -0.48863
H    -2.18313    +0.26150    -0.58358


* E =  +1.894 kcal/mol ; Conformer 028
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49852
C    +1.38433    +0.00000    +2.12562
C    +2.22578    -1.21880    +1.79257
C    +1.68855    -2.53325    +2.27484
O    +0.94745    -2.41218    +3.37669
C    +0.45526    -3.62896    +3.90913
O    +1.92157    -3.59552    +1.76607
H    -0.12355    -3.35843    +4.78282
H    -0.16685    -4.13705    +3.17901
H    +1.27777    -4.28256    +4.18231
H    +2.39109    -1.32652    +0.72435
H    +3.21278    -1.11739    +2.24575
H    +1.92533    +0.88580    +1.79160
H    +1.28593    +0.07983    +3.20580
H    -0.53594    +0.88444    +1.85171
H    -0.57062    -0.85339    +1.86858
H    +0.29648    -1.26288    -0.42443
H    -0.97009    +0.13215    -0.46565
H    +0.77050    +0.59874    -0.47670
H    +0.45769    -2.12247    -0.68135


* E =  +1.973 kcal/mol ; Conformer 029
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49708
C    +1.38523    +0.00000    +2.12384
C    +2.17757    -1.26307    +1.81990
C    +3.49807    -1.30981    +2.52205
O    +4.22710    -0.22150    +2.27988
C    +5.49958    -0.19208    +2.90108
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O    +3.88420    -2.20798    +3.22034
H    +5.95166    +0.74617    +2.60684
H    +5.39550    -0.24493    +3.98027
H    +6.10381    -1.02946    +2.56625
H    +1.62948    -2.15306    +2.11570
H    +2.37848    -1.33303    +0.75131
H    +1.94590    +0.86705    +1.77975
H    +1.28129    +0.10096    +3.20366
H    -0.54677    +0.87288    +1.85271
H    -0.55895    -0.86886    +1.85919
H    +0.65763    +1.14487    -0.37566
H    +0.58457    -0.77118    -0.48930
H    -0.96689    +0.13782    -0.47006
H    +1.08412    +1.91913    -0.58394

* E =  +1.992 kcal/mol ; Conformer 030
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49723
C    +1.38456    +0.00000    +2.12514
C    +2.16830    -1.27288    +1.84198
C    +3.50411    -1.30919    +2.51706
O    +3.40655    -1.08171    +3.82657
C    +4.62934    -1.11432    +4.54059
O    +4.55288    -1.52642    +1.97333
H    +4.37589    -0.91080    +5.57291
H    +5.09678    -2.08955    +4.44654
H    +5.31103    -0.36110    +4.15832
H    +1.59956    -2.13406    +2.19612
H    +2.35473    -1.41045    +0.78225
H    +1.94497    +0.86064    +1.75903
H    +1.29166    +0.11896    +3.20205
H    -0.54795    +0.87255    +1.85204
H    -0.55775    -0.86916    +1.86115
H    +0.63384    +1.15837    -0.37040
H    +0.60195    -0.75703    -0.48995
H    -0.96896    +0.12003    -0.47064
H    +1.04388    +1.94408    -0.57117

* E =  +2.148 kcal/mol ; Conformer 031
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49707
C    +1.38089    +0.00000    +2.13512
C    +2.22463    +1.20987    +1.76997
C    +2.98889    +1.03574    +0.49247
O    +3.18699    +2.19571    -0.13199
C    +3.96140    +2.12034    -1.31630
O    +3.41246    -0.00800    +0.07656
H    +3.48123    +1.47126    -2.04184
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H    +4.02589    +3.13283    -1.69307
H    +4.95031    +1.72953    -1.09797
H    +1.63283    +2.12103    +1.71098
H    +2.98119    +1.38459    +2.53579
H    +1.26104    -0.03254    +3.21601
H    +1.92352    -0.89865    +1.84528
H    -0.55545    +0.87326    +1.85555
H    -0.55236    -0.86918    +1.85378
H    +0.65106    -1.15174    -0.38132
H    -0.97019    -0.13128    -0.46548
H    +0.58064    +0.77559    -0.48846
H    +1.05756    -1.93061    -0.58982


* E =   +2.599 kcal/mol ; Conformer 032
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49706
C    +1.37112    +0.00000    +2.15533
C    +2.17336    +1.27939    +1.98231
C    +2.95724    +1.46448    +0.71665
O    +3.13092    +0.33837    +0.02826
C    +3.87890    +0.47683    -1.16676
O    +3.42939    +2.51357    +0.37139
H    +3.93045    -0.51303    -1.60185
H    +3.38194    +1.16756    -1.84112
H    +4.87379    +0.85254    -0.94989
H    +1.54434    +2.16219    +2.08114
H    +2.91585    +1.35894    +2.77694
H    +1.22681    -0.15568    +3.22326
H    +1.95308    -0.84667    +1.79521
H    -0.57851    +0.85101    +1.86247
H    -0.53889    -0.88775    +1.83962
H    +0.40780    +1.23270    -0.42952
H    +0.72016    -0.65827    -0.47230
H    -0.98090    -0.04568    -0.46016
H    +0.63565    +2.06910    -0.71011


* E =   +7.839 kcal/mol ; Conformer 033
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49748
C    +1.38469    +0.00000    +2.12545
C    +2.25051    -1.17448    +1.71366
C    +1.69630    -2.48903    +2.19553
O    +2.22205    -3.61371    +1.69919
C    +3.20854    -3.57983    +0.69360
O    +0.83715    -2.57075    +3.02581
H    +3.52318    -4.60693    +0.55632
H    +2.80190    -3.20424    -0.24287
H    +4.06745    -2.98240    +0.99028
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H    +2.38852    -1.19802    +0.63488
H    +3.25048    -1.07210    +2.13993
H    +1.90547    +0.91789    +1.85159
H    +1.28058    -0.00202    +3.20772
H    -0.53347    +0.88746    +1.84714
H    -0.56643    -0.85232    +1.86948
H    +0.32928    -1.25823    -0.42058
H    -0.97289    +0.10070    -0.46746
H    +0.75591    +0.61299    -0.48319
H    +0.52284    -2.11317    -0.67513


* E =  +8.044 kcal/mol ; Conformer 034
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49525
C    +1.40217    +0.00000    +2.07687
C    +1.41776    -0.00025    +3.59103
C    +0.97039    +1.31532    +4.17106
O    +0.80964    +1.39069    +5.49803
C    +1.01543    +0.27092    +6.32777
O    +0.77426    +2.29421    +3.51110
H    +0.90544    +0.63279    +7.34242
H    +0.27206    -0.50203    +6.14586
H    +2.01274    -0.14484    +6.20637
H    +0.79375    -0.80423    +3.98242
H    +2.42397    -0.19701    +3.96457
H    +1.93871    -0.87835    +1.72020
H    +1.94007    +0.87609    +1.71900
H    -0.53414    +0.88117    +1.85726
H    -0.54917    -0.87065    +1.85976
H    +0.61515    -1.16906    -0.37315
H    -0.96785    -0.09518    -0.47843
H    +0.62700    +0.75029    -0.47018
H    +1.01711    -1.96073    -0.56748


* E =  +8.150 kcal/mol ; Conformer 035
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49750
C    +1.37688    +0.00000    +2.14369
C    +2.22706    +1.20289    +1.77438
C    +3.01434    +1.00061    +0.50457
O    +3.60479    +2.06779    -0.04171
C    +3.39363    +3.36452    +0.46719
O    +3.17782    -0.07092    -0.00466
H    +4.04746    +4.01301    -0.10262
H    +2.36289    +3.67979    +0.31914
H    +3.65520    +3.43357    +1.52050
H    +1.61322    +2.09919    +1.69795
H    +2.96045    +1.40698    +2.55708
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H    +1.24844    -0.01971    +3.22413
H    +1.91627    -0.90311    +1.86606
H    -0.57327    +0.85663    +1.85985
H    -0.54204    -0.88276    +1.84685
H    +0.39204    +1.24580    -0.40953
H    +0.73340    -0.63701    -0.47998
H    -0.98025    -0.04557    -0.46123
H    +0.61209    +2.09752    -0.65246


* E =   +8.266 kcal/mol ; Conformer 036
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49795
C    +1.38170    +0.00000    +2.12738
C    +2.20052    -1.22001    +1.76579
C    +3.51521    -1.24754    +2.49412
O    +4.32356    -2.29389    +2.28036
C    +3.94911    -3.34324    +1.41785
O    +3.87166    -0.38566    +3.24373
H    +4.78621    -4.03004    +1.41014
H    +3.06653    -3.86477    +1.78100
H    +3.77117    -2.98940    +0.40519
H    +1.64833    -2.13464    +1.98909
H    +2.39795    -1.25760    +0.69425
H    +1.92693    +0.89412    +1.82837
H    +1.29447    +0.05612    +3.20983
H    -0.53809    +0.88470    +1.84699
H    -0.57593    -0.85373    +1.86162
H    +0.32339    -1.26064    -0.42545
H    -0.97051    +0.11213    -0.46993
H    +0.76297    +0.60891    -0.47586
H    +0.50680    -2.11213    -0.68854


* E =   +8.430 kcal/mol ; Conformer 037
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49584
C    +1.41034    +0.00000    +2.07135
C    +1.42669    +0.00625    +3.58661
C    +0.99265    +1.33010    +4.15860
O    +0.81823    +1.41117    +5.48338
C    +0.99066    +0.28887    +6.31726
O    +0.82124    +2.31005    +3.49376
H    +0.88102    +0.65575    +7.33015
H    +0.23031    -0.46632    +6.13100
H    +1.97877    -0.15083    +6.20506
H    +0.79529    -0.79005    +3.98138
H    +2.43156    -0.19679    +3.96087
H    +1.94564    -0.88129    +1.71969
H    +1.94932    +0.87305    +1.70939
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H   -0.52919   +0.87736   +1.86304
H   -0.53423   -0.87864   +1.86223
H   -1.31650   -0.03932   -0.38908
H   +0.34548   +0.91396   -0.47047
H   +0.39756   -0.89035   -0.47635
H   -2.19296   -0.07079   -0.60850


* E =  +8.483 kcal/mol ; Conformer 038
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49617
C   +1.40752   +0.00000   +2.07512
C   +1.40050   -0.00009   +3.58813
C   +2.79245   +0.00016   +4.15789
O   +2.92193   -0.00019   +5.49124
C   +1.79561   -0.00103   +6.33676
O   +3.77883   +0.00069   +3.48151
H   +2.18594   -0.00104   +7.34677
H   +1.18491   +0.88752   +6.19398
H   +1.18594   -0.89022   +6.19357
H   +0.86290   +0.86934   +3.97025
H   +0.86321   -0.86974   +3.97018
H   +1.96014   -0.86801   +1.72089
H   +1.96012   +0.86808   +1.72101
H   -0.54169   +0.87402   +1.86111
H   -0.54171   -0.87401   +1.86112
H   -1.31921   -0.00000   -0.38593
H   +0.37305   +0.90180   -0.47319
H   +0.37305   -0.90179   -0.47319
H   -2.19756   +0.00003   -0.59702


* E =  +8.571 kcal/mol ; Conformer 039
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49609
C   +1.39935   +0.00000   +2.08132
C   +1.38959   -0.02119   +3.59321
C   +2.77847   +0.02017   +4.16863
O   +2.90420   -0.03280   +5.50167
C   +1.77843   -0.14628   +6.33997
O   +3.76542   +0.10338   +3.49849
H   +2.16305   -0.13706   +7.35217
H   +1.09535   +0.69057   +6.21393
H   +1.24660   -1.08025   +6.17279
H   +0.82569   +0.82710   +3.98624
H   +0.87761   -0.91107   +3.96246
H   +1.95625   -0.86013   +1.71411
H   +1.94807   +0.87631   +1.74077
H   -0.54711   +0.87640   +1.85879
H   -0.55577   -0.86707   +1.85840
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H    +0.56589    -1.19254    -0.36885
H    -0.97076    -0.05838    -0.47841
H    +0.65822    +0.72142    -0.47254
H    +0.93018    -2.00161    -0.56239

* E =   +8.613 kcal/mol ; Conformer 040
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49591
C    +1.40154    +0.00000    +2.07965
C    +1.41990    -0.10147    +3.59061
C    +0.91450    +1.14827    +4.26129
O    +0.75839    +1.12283    +5.59142
C    +1.02350    -0.04000    +6.34075
O    +0.66817    +2.15989    +3.67232
H    +0.89955    +0.24416    +7.37830
H    +0.31935    -0.83521    +6.10605
H    +2.04005    -0.39551    +6.19039
H    +0.83328    -0.95765    +3.92550
H    +2.43487    -0.27788    +3.95038
H    +1.96319    -0.84005    +1.67072
H    +1.91537    +0.91003    +1.77623
H    -0.54421    +0.86694    +1.86618
H    -0.53931    -0.88404    +1.85438
H    +0.64054    +1.15130    -0.38589
H    +0.61068    -0.76232    -0.47385
H    -0.96633    +0.11522    -0.47694
H    +1.06402    +1.92095    -0.61182

* E =   +8.785 kcal/mol ; Conformer 041
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49690
C    +1.38644    +0.00000    +2.12346
C    +2.20228    -1.24576    +1.83939
C    +1.65184    -2.46475    +2.53019
O    +2.20823    -3.64913    +2.24577
C    +3.25658    -3.76325    +1.31177
O    +0.76275    -2.42454    +3.33030
H    +3.57058    -4.79898    +1.34730
H    +2.91994    -3.53086    +0.30382
H    +4.10033    -3.12833    +1.57096
H    +2.28199    -1.43482    +0.76973
H    +3.22806    -1.10935    +2.18604
H    +1.94193    +0.86496    +1.76259
H    +1.28502    +0.10502    +3.20094
H    -0.53930    +0.87810    +1.85042
H    -0.55739    -0.86191    +1.87002
H    +0.67110    +1.13454    -0.38006
H    +0.57407    -0.77758    -0.49318
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H   -0.96561   +0.14623   -0.47025
H   +1.11252   +1.90218   -0.58975


* E =  +8.981 kcal/mol ; Conformer 042
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49795
C   +1.39476   +0.00000   +2.11253
C   +2.19322   -1.23961   +1.77293
C   +3.52929   -1.25151   +2.46315
O   +4.33191   -2.30343   +2.25286
C   +3.94209   -3.36675   +1.41592
O   +3.90514   -0.37348   +3.18316
H   +4.76894   -4.06586   +1.42390
H   +3.05230   -3.86776   +1.79032
H   +3.77135   -3.03329   +0.39484
H   +1.64244   -2.13905   +2.05507
H   +2.35596   -1.31817   +0.69736
H   +1.94745   +0.87948   +1.78690
H   +1.31728   +0.08149   +3.19464
H   -0.52931   +0.88275   +1.85506
H   -0.55887   -0.86207   +1.86466
H   -1.30509   +0.15508   -0.37864
H   +0.47057   +0.85789   -0.46949
H   +0.25655   -0.93308   -0.48989
H   -2.18078   +0.26637   -0.58667


* E =  +9.067 kcal/mol ; Conformer 043
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49796
C   +1.39822   +0.00000   +2.10962
C   +2.22046   -1.22900   +1.77699
C   +1.69804   -2.46972   +2.45083
O   +2.25236   -3.64228   +2.11745
C   +3.27132   -3.72420   +1.14832
O   +0.83421   -2.45628   +3.27872
H   +3.59278   -4.75825   +1.14631
H   +2.90162   -3.46756   +0.15800
H   +4.11889   -3.09042   +1.39784
H   +2.26986   -1.38747   +0.70019
H   +3.25336   -1.09221   +2.10167
H   +1.94145   +0.88010   +1.76630
H   +1.30744   +0.07569   +3.19102
H   -0.52136   +0.88781   +1.85462
H   -0.55235   -0.85720   +1.87687
H   -1.30009   +0.17477   -0.38024
H   +0.48252   +0.84918   -0.47427
H   +0.23742   -0.93736   -0.49170
H   -2.17232   +0.30188   -0.59836
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* E =  +9.209 kcal/mol ; Conformer 044
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49763
C   +1.38177   +0.00000   +2.13038
C   +2.19161   -1.23655   +1.80466
C   +3.49326   -1.26731   +2.55835
O   +4.32375   -2.29338   +2.32764
C   +4.00820   -3.29639   +1.39112
O   +3.81559   -0.43154   +3.35059
H   +4.82317   -4.00800   +1.43620
H   +3.08038   -3.80559   +1.64142
H   +3.94471   -2.89613   +0.38167
H   +1.62817   -2.13950   +2.05015
H   +2.40588   -1.30165   +0.73802
H   +1.93528   +0.88193   +1.81277
H   +1.29035   +0.07857   +3.21089
H   -0.54755   +0.87206   +1.85290
H   -0.56223   -0.86856   +1.85727
H   +0.69209   +1.12301   -0.38023
H   +0.56243   -0.78829   -0.48890
H   -0.96200   +0.16394   -0.47175
H   +1.14533   +1.87941   -0.59802

* E =  +9.603 kcal/mol ; Conformer 045
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49687
C   +1.39031   +0.00000   +2.12709
C   +2.23428   -1.19965   +1.73795
C   +2.97838   -1.00123   +0.44290
O   +3.55913   -2.07177   -0.11368
C   +3.45923   -3.35123   +0.46758
O   +3.10668   +0.06261   -0.08936
H   +4.11162   -3.98989   -0.11481
H   +3.79330   -3.35305   +1.50227
H   +2.44393   -3.73730   +0.40956
H   +2.98996   -1.39856   +2.50025
H   +1.62248   -2.10022   +1.68631
H   +1.92391   +0.90561   +1.84774
H   +1.27429   +0.01131   +3.20961
H   -0.53457   +0.87900   +1.85640
H   -0.55399   -0.86669   +1.86185
H   -1.31640   +0.12805   -0.36915
H   +0.46517   +0.85672   -0.47282
H   +0.27236   -0.93076   -0.48689
H   -2.19456   +0.22061   -0.56737

* E =  +9.993 kcal/mol ; Conformer 046
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```
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49745
C    +1.39037    +0.00000    +2.11897
C    +2.29658    +1.13742    +1.64491
C    +1.66412    +2.47938    +1.88510
O    +1.84907    +3.08338    +3.06559
C    +2.74868    +2.57385    +4.02330
O    +0.95127    +3.00452    +1.07786
H    +2.63179    +3.20084    +4.89857
H    +2.51907    +1.54582    +4.29107
H    +3.77658    +2.64265    +3.67451
H    +3.26915    +1.05455    +2.12201
H    +2.44945    +1.05977    +0.57297
H    +1.29218    +0.02777    +3.20399
H    +1.88984    -0.93668    +1.87608
H    -0.55615    +0.87530    +1.84416
H    -0.53749    -0.87098    +1.86933
H    +0.89041    -0.97986    -0.39089
H    -0.91798    -0.33147    -0.47062
H    +0.40846    +0.88869    -0.46716
H    +1.48730    -1.62554    -0.61319

* E = +10.004 kcal/mol ; Conformer 047
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49583
C    +1.40002    +0.00000    +2.08018
C    +1.38861    -0.01458    +3.60464
C    +2.78881    +0.06965    +4.14691
O    +3.46994    -1.06364    +4.35890
C    +2.86924    -2.32840    +4.20111
O    +3.33411    +1.11571    +4.34852
H    +3.66654    -3.05013    +4.32894
H    +2.11031    -2.50268    +4.96060
H    +2.43593    -2.45255    +3.21183
H    +0.86958    +0.86586    +3.97183
H    +0.85878    -0.89186    +3.96844
H    +1.94882    -0.86049    +1.69556
H    +1.93949    +0.88480    +1.74440
H    -0.54196    +0.87673    +1.86275
H    -0.55295    -0.86723    +1.86091
H    +0.58760    -1.18393    -0.36400
H    -0.96953    -0.07606    -0.47806
H    +0.64527    +0.73238    -0.47346
H    +0.97104    -1.98729    -0.54625

* E = +10.085 kcal/mol ; Conformer 048
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49557
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C    +1.40445    +0.00000    +2.07191
C    +1.43623    -0.01602    +3.60013
C    +0.81483    +1.22703    +4.17351
O    +1.58033    +2.31494    +4.33519
C    +2.97725    +2.27147    +4.15520
O    -0.35035    +1.30190    +4.43924
H    +3.31956    +3.29282    +4.26756
H    +3.45345    +1.65445    +4.91393
H    +3.25066    +1.91341    +3.16606
H    +0.84265    -0.84861    +3.96586
H    +2.45567    -0.15286    +3.95033
H    +1.93903    -0.87815    +1.71199
H    +1.94848    +0.86654    +1.69230
H    -0.55325    +0.86664    +1.86455
H    -0.54338    -0.87015    +1.86556
H    +0.62497    -1.16251    -0.37588
H    -0.96820    -0.10241    -0.47577
H    +0.61996    +0.75376    -0.47497
H    +1.03766    -1.94771    -0.57374

* E = +10.093 kcal/mol ; Conformer 049
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49565
C    +1.40526    +0.00000    +2.07013
C    +1.44291    +0.06800    +3.59634
C    +0.74641    -1.10975    +4.22073
O    +1.43812    -2.23913    +4.41946
C    +2.83148    -2.30024    +4.21762
O    -0.41783    -1.09311    +4.50036
H    +3.10418    -3.33774    +4.36628
H    +3.11155    -2.00217    +3.21084
H    +3.36186    -1.68852    +4.94407
H    +2.47043    +0.15409    +3.93967
H    +0.90277    +0.94799    +3.93293
H    +1.93402    -0.88486    +1.71437
H    +1.95373    +0.85882    +1.68337
H    -0.53850    +0.87809    +1.86415
H    -0.55840    -0.85794    +1.86718
H    +0.62890    -1.16007    -0.37359
H    -0.96740    -0.10788    -0.47608
H    +0.61886    +0.75366    -0.47674
H    +1.04734    -1.94233    -0.57244

* E = +10.169 kcal/mol ; Conformer 050
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49817
C    +1.38705    +0.00000    +2.12367
C    +2.25593    -1.16521    +1.66107
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C   +3.55282   -1.18109   +2.42222
O   +4.59157   -0.48804   +1.94058
C   +4.54250   +0.13873   +0.67823
O   +3.67280   -1.74853   +3.46934
H   +5.45667   +0.71427   +0.60113
H   +4.51877   -0.59534   -0.12419
H   +3.69212   +0.80950   +0.58571
H   +1.75816   -2.10407   +1.88771
H   +2.41908   -1.11816   +0.58752
H   +1.88027   +0.94468   +1.89273
H   +1.29436   -0.04713   +3.20679
H   -0.54538   +0.86813   +1.86404
H   -0.55096   -0.87589   +1.85407
H   +0.91371   +0.95280   -0.38846
H   +0.40336   -0.88416   -0.48149
H   -0.90957   +0.34418   -0.47754
H   +1.54070   +1.57039   -0.61524

* E = +10.226 kcal/mol ; Conformer 051
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49610
C   +1.40711   +0.00000   +2.07678
C   +1.39546   -0.02143   +3.60250
C   +2.79845   -0.09192   +4.13896
O   +3.45473   +1.04915   +4.38760
C   +2.82399   +2.30387   +4.27783
O   +3.36873   -1.13114   +4.30225
H   +3.60386   +3.03936   +4.43210
H   +2.38645   +2.45426   +3.29382
H   +2.06167   +2.43186   +5.04309
H   +0.84820   +0.83580   +3.98721
H   +0.89386   -0.92084   +3.94684
H   +1.95488   -0.87127   +1.72130
H   +1.94931   +0.87447   +1.71458
H   -0.54144   +0.87237   +1.86447
H   -0.53497   -0.87583   +1.86427
H   -1.31754   -0.00026   -0.38456
H   +0.37117   +0.90197   -0.47470
H   +0.37270   -0.90198   -0.47289
H   -2.19618   +0.00063   -0.59750

* E = +10.242 kcal/mol ; Conformer 052
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49706
C   +1.40003   +0.00000   +2.10358
C   +2.27635   -1.17308   +1.66019
C   +1.61698   -2.49247   +1.95016
O   +1.79797   -3.06067   +3.14876
```

```
C   +2.71571   -2.53933   +4.08250
O   +0.88872   -3.02873   +1.16462
H   +2.59167   -3.13363   +4.97932
H   +3.73923   -2.64279   +3.72930
H   +2.51083   -1.49800   +4.31696
H   +2.41307   -1.13749   +0.58378
H   +3.25669   -1.09772   +2.12269
H   +1.91545   +0.91848   +1.82464
H   +1.31300   +0.01336   +3.19042
H   -0.52307   +0.88187   +1.86699
H   -0.55458   -0.86653   +1.85411
H   -1.30122   +0.20732   -0.37216
H   +0.49741   +0.84073   -0.47413
H   +0.21871   -0.95134   -0.47052
H   -2.17002   +0.36319   -0.57486


* E = +10.352 kcal/mol ; Conformer 053
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49609
C   +1.39851   +0.00000   +2.08432
C   +1.38068   -0.00571   +3.60903
C   +2.77933   -0.06238   +4.15858
O   +3.43334   +1.08602   +4.38076
C   +2.80037   +2.33641   +4.24089
O   +3.34841   -1.09579   +4.35729
H   +3.57856   +3.07700   +4.37867
H   +2.36313   +2.46325   +3.25351
H   +2.03714   +2.48072   +5.00243
H   +0.82778   +0.85326   +3.98260
H   +0.88126   -0.90334   +3.96106
H   +1.94299   -0.87667   +1.73690
H   +1.94561   +0.86908   +1.71519
H   -0.54733   +0.87497   +1.86120
H   -0.54861   -0.86876   +1.86252
H   +0.59948   -1.17526   -0.37380
H   -0.96967   -0.08392   -0.47648
H   +0.63581   +0.74074   -0.47380
H   +0.98993   -1.96949   -0.57509


* E = +10.374 kcal/mol ; Conformer 054
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49777
C   +1.38197   +0.00000   +2.12676
C   +2.19260   +1.24972   +1.79588
C   +3.47766   +1.25440   +2.57635
O   +4.57397   +0.71800   +2.02357
C   +4.57861   +0.25294   +0.69397
O   +3.54515   +1.67460   +3.69493
```

```
H    +5.54588    -0.21226    +0.54880
H    +3.80101    -0.48728    +0.52029
H    +4.47034    +1.07228    -0.01302
H    +2.35984    +1.33082    +0.72610
H    +1.64069    +2.13050    +2.11183
H    +1.28745    -0.06925    +3.20862
H    +1.92255    -0.89219    +1.80497
H    -0.57008    +0.85519    +1.86491
H    -0.53711    -0.88453    +1.84906
H    +0.32159    +1.25889    -0.43322
H    +0.76011    -0.61277    -0.47604
H    -0.97147    -0.11461    -0.46704
H    +0.50167    +2.10612    -0.70783

* E = +10.378 kcal/mol ; Conformer 055
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49782
C    +1.38529    +0.00000    +2.12020
C    +2.22787    -1.20559    +1.71248
C    +3.56493    -1.15374    +2.39711
O    +3.70523    -1.74798    +3.59006
C    +2.67174    -2.51969    +4.15612
O    +4.49490    -0.55431    +1.94095
H    +3.01558    -2.78980    +5.14701
H    +1.74577    -1.95640    +4.24473
H    +2.49599    -3.42741    +3.58329
H    +1.69017    -2.12872    +1.91599
H    +2.43190    -1.17208    +0.64736
H    +1.91964    +0.90419    +1.83062
H    +1.28735    +0.03644    +3.20540
H    -0.53666    +0.88296    +1.85321
H    -0.57052    -0.85720    +1.86177
H    +0.29144    -1.27046    -0.41488
H    -0.96902    +0.13460    -0.46657
H    +0.77692    +0.58910    -0.47728
H    +0.44812    -2.13156    -0.66063

* E = +10.560 kcal/mol ; Conformer 056
C    +0.00000    +0.00000    +0.00000
C    +0.00000    +0.00000    +1.49693
C    +1.37881    +0.00000    +2.13960
C    +2.18404    -1.26120    +1.87518
C    +3.03308    -1.18595    +0.63309
O    +3.63364    -2.31175    +0.22258
C    +3.45405    -3.53376    +0.89954
O    +3.22191    -0.17788    +0.01859
H    +4.12440    -4.23628    +0.42011
H    +3.71638    -3.45647    +1.95195
```

```
H    +2.43357   -3.89785   +0.80255
H    +2.86881   -1.45543   +2.70271
H    +1.53086   -2.13295   +1.82631
H    +1.94784   +0.85882   +1.78931
H    +1.25399   +0.11004   +3.21499
H    -0.54836   +0.87377   +1.84950
H    -0.56160   -0.86661   +1.86320
H    +0.59417   +1.18252   -0.36384
H    +0.63262   -0.72584   -0.49680
H    -0.97654   +0.08405   -0.46326
H    +0.96264   +1.98698   -0.54752

* E = +10.610 kcal/mol ; Conformer 057
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49652
C    +1.41367   +0.00000   +2.06384
C    +1.45463   +0.03010   +3.59286
C    +0.83374   -1.20498   +4.18398
O    +1.59600   -2.29571   +4.34385
C    +2.99130   -2.25946   +4.15166
O    -0.32761   -1.27075   +4.46669
H    +3.33051   -3.28124   +4.26944
H    +3.25800   -1.91072   +3.15734
H    +3.47657   -1.63831   +4.90129
H    +2.47722   +0.16671   +3.93444
H    +0.86610   +0.86811   +3.95424
H    +1.95275   -0.87089   +1.68880
H    +1.95080   +0.87338   +1.69567
H    -0.52894   +0.87768   +1.86840
H    -0.54640   -0.86389   +1.87081
H    -1.31592   +0.03182   -0.38991
H    +0.39280   +0.89246   -0.47606
H    +0.34912   -0.91090   -0.47473
H    -2.19089   +0.05588   -0.61450

* E = +10.678 kcal/mol ; Conformer 058
C    +0.00000   +0.00000   +0.00000
C    +0.00000   +0.00000   +1.49756
C    +1.39547   +0.00000   +2.11132
C    +2.19157   +1.25862   +1.77983
C    +3.50306   +1.25801   +2.51528
O    +4.57238   +0.70205   +1.93039
C    +4.53033   +0.23955   +0.60043
O    +3.61409   +1.68996   +3.62572
H    +5.48206   -0.24790   +0.42848
H    +3.73086   -0.48089   +0.44506
H    +4.42380   +1.06373   -0.10141
H    +2.32512   +1.35648   +0.70581
```

```
H   +1.64759   +2.13058   +2.13183
H   +1.31153   -0.07664   +3.19407
H   +1.93661   -0.88672   +1.77790
H   -0.55163   +0.86482   +1.86645
H   -0.52999   -0.88143   +1.85724
H   -1.30579   -0.14612   -0.37815
H   +0.26325   +0.93135   -0.48889
H   +0.46145   -0.86249   -0.47063
H   -2.18131   -0.25282   -0.58808

* E = +10.716 kcal/mol ; Conformer 059
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49734
C   +1.39688   +0.00000   +2.10823
C   +2.20907   -1.23801   +1.73992
C   +3.56923   -1.17930   +2.37792
O   +3.73609   -1.70841   +3.59745
C   +2.70665   -2.42291   +4.24071
O   +4.49647   -0.63055   +1.85729
H   +3.07705   -2.64103   +5.23480
H   +1.79506   -1.83609   +4.32443
H   +2.49560   -3.35945   +3.72933
H   +1.66375   -2.13929   +2.01142
H   +2.38075   -1.25972   +0.66851
H   +1.94474   +0.88210   +1.77995
H   +1.30695   +0.07808   +3.19236
H   -0.52800   +0.88286   +1.85691
H   -0.55548   -0.86353   +1.86523
H   -1.30741   +0.16049   -0.37459
H   +0.47302   +0.85624   -0.46934
H   +0.25344   -0.93386   -0.48877
H   -2.18201   +0.27610   -0.57885

* E = +11.031 kcal/mol ; Conformer 060
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49713
C   +1.38604   +0.00000   +2.12157
C   +2.18293   -1.26632   +1.81745
C   +3.51859   -1.22103   +2.50672
O   +3.61432   -1.68930   +3.75907
C   +2.54115   -2.35237   +4.38534
O   +4.48676   -0.73479   +1.99947
H   +2.86037   -2.53049   +5.40487
H   +1.63898   -1.74561   +4.39884
H   +2.33427   -3.30790   +3.90841
H   +1.60793   -2.14697   +2.09607
H   +2.39879   -1.32777   +0.75614
H   +1.95147   +0.85985   +1.76539
```

```
H   +1.28685   +0.12153   +3.20022
H   -0.54492   +0.87420   +1.85259
H   -0.55931   -0.86785   +1.86195
H   +0.62800   +1.16154   -0.37108
H   +0.60310   -0.75591   -0.49006
H   -0.97048   +0.11574   -0.46829
H   +1.03152   +1.94971   -0.57176


*  E = +11.207 kcal/mol ; Conformer 061
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49778
C   +1.38663   +0.00000   +2.12108
C   +2.16913   +1.29965   +1.91851
C   +1.48902   +2.44195   +2.61903
O   +1.80332   +2.69501   +3.89826
C   +2.85430   +2.02177   +4.55084
O   +0.63308   +3.09899   +2.10072
H   +2.82520   +2.35927   +5.57964
H   +2.72290   +0.94267   +4.52922
H   +3.81904   +2.28282   +4.12143
H   +3.19297   +1.17014   +2.25744
H   +2.19702   +1.55751   +0.86483
H   +1.29805   -0.21017   +3.18721
H   +1.97076   -0.81609   +1.69562
H   -0.57781   +0.84783   +1.86453
H   -0.52424   -0.89483   +1.84438
H   +0.38602   +1.23417   -0.47319
H   +0.72287   -0.65824   -0.47336
H   -0.97903   -0.06805   -0.46007
H   +0.61317   +2.04063   -0.81128


*  E = +11.443 kcal/mol ; Conformer 062
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49834
C   +1.39434   +0.00000   +2.11768
C   +1.98928   -1.39310   +2.34067
C   +1.93047   -2.25944   +1.11437
O   +2.88801   -2.13828   +0.18587
C   +4.05073   -1.37606   +0.42123
O   +1.02468   -3.01575   +0.90891
H   +4.60650   -1.39381   -0.50798
H   +3.81797   -0.34560   +0.67407
H   +4.65926   -1.82118   +1.20518
H   +3.00516   -1.30350   +2.71815
H   +1.39972   -1.91387   +3.08889
H   +2.05579   +0.60862   +1.50153
H   +1.36238   +0.48337   +3.09204
H   -0.54309   +0.87763   +1.84672
```

```
H   -0.55917   -0.86768   +1.85950
H   +0.61729   +1.17308   -0.35954
H   +0.61262   -0.74445   -0.49502
H   -0.97238   +0.10564   -0.46689
H   +1.02726   +1.96394   -0.54035


* E = +11.785 kcal/mol ; Conformer 063
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49955
C   +1.39546   +0.00000   +2.12572
C   +2.03453   +1.38271   +2.26831
C   +2.05081   +2.17272   +0.98968
O   +3.03406   +1.95996   +0.10626
C   +4.15341   +1.16568   +0.42614
O   +1.19082   +2.95939   +0.71302
H   +4.73679   +1.09952   -0.48385
H   +4.75841   +1.63348   +1.19966
H   +3.86820   +0.16457   +0.73695
H   +1.44425   +1.97324   +2.96224
H   +3.03472   +1.28233   +2.68371
H   +1.33810   -0.42042   +3.12872
H   +2.04289   -0.66685   +1.55625
H   -0.56242   +0.85761   +1.86769
H   -0.52267   -0.89077   +1.84767
H   -1.29048   -0.23888   -0.36499
H   +0.19923   +0.94181   -0.49429
H   +0.50965   -0.83980   -0.46223
H   -2.15937   -0.42479   -0.56205


* E = +12.154 kcal/mol ; Conformer 064
C   +0.00000   +0.00000   +0.00000
C   +0.00000   +0.00000   +1.49668
C   +1.38867   +0.00000   +2.11698
C   +2.20549   -1.26370   +1.80080
C   +3.13674   -1.09456   +0.63156
O   +4.25524   -0.38125   +0.82032
C   +4.68329   -0.00365   +2.10884
O   +2.91686   -1.53740   -0.45877
H   +5.54989   +0.62785   +1.95690
H   +3.92537   +0.55930   +2.64670
H   +4.97831   -0.87267   +2.69330
H   +2.77735   -1.56796   +2.67460
H   +1.54289   -2.08603   +1.54742
H   +1.92111   +0.88966   +1.77973
H   +1.28718   +0.09145   +3.19671
H   -0.54597   +0.87010   +1.86156
H   -0.54943   -0.87291   +1.86348
H   +0.63789   +1.15984   -0.35791
```

```
H   +0.60894   -0.75321   -0.48648
H   -0.97000   +0.12771   -0.46627
H   +1.05007   +1.95105   -0.53422
```

S.3. Scaled Vibrational Frequencies

Vibrational frequencies for all structures at the MPWB1K/6-31+G(d,p) level

S.3.1 Methyl Pentanoate

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==========================
       Structure    1
==========================


     35.3664      72.6927     103.0518     138.4946     171.6618     207.1096
    240.2512     248.6141     298.4475     355.9804     508.8580     572.3890
    643.6802     727.0313     826.4585     832.1250     903.2286     922.4480
   1000.5941    1038.3569    1052.4558    1092.5487    1115.1181    1148.3548
   1175.2698    1194.7123    1228.6843    1249.7998    1285.6510    1294.0600
   1365.7165    1375.2857    1380.8817    1414.5495    1435.1774    1440.3502
   1444.0875    1448.9559    1455.2755    1457.7962    1461.3740    1799.7239
   2953.2472    2958.4071    2966.5384    2977.2054    2987.5213    3002.2907
   3017.5002    3026.6462    3037.2387    3042.7339    3070.7396    3103.6246


==========================
       Structure    2
==========================


     28.9145      66.9109     101.8277     115.6596     135.5822     173.2454
    238.5680     250.5845     300.4398     338.3697     475.8559     569.8975
    689.5433     708.4014     779.6823     880.7592     907.7988     911.5259
   1013.1212    1043.5694    1064.1965    1096.9065    1114.8467    1148.3603
   1174.6343    1195.4726    1206.2345    1270.6187    1272.0407    1286.4250
   1347.0098    1377.6096    1391.7968    1416.2550    1439.2853    1443.8311
   1444.2639    1451.3225    1454.8856    1458.0904    1464.4494    1802.9868
   2948.3722    2960.3161    2969.5040    2976.5926    2982.1862    2987.2111
   3006.2809    3026.3730    3037.2018    3043.1449    3070.3258    3102.9154


==========================
       Structure    3
==========================


     32.6511      50.6526     115.8413     140.8795     173.2882     190.6321
    258.0006     271.6806     341.5745     386.1386     472.0116     574.2712
    647.3149     737.1185     815.5147     834.8080     902.0515     931.8825
    965.0255    1036.9013    1056.9398    1080.0186    1117.7307    1148.4065
   1172.7838    1179.2469    1219.9458    1246.5726    1281.9533    1329.2921
```

1355.9637	1375.6449	1380.8620	1417.0313	1433.1646	1440.5326
1444.0153	1449.7684	1457.7464	1458.4358	1464.0266	1799.3162
2958.2703	2966.2860	2971.7605	2981.0657	2987.3396	3010.7744
3020.8317	3035.1263	3037.8102	3042.2606	3070.5147	3103.3657

===========================
Structure   4
===========================

25.6240	57.7862	103.4400	135.9477	138.2032	171.5125
232.7792	274.8168	305.5469	408.6856	432.2551	571.0713
686.7956	732.5295	776.2857	867.9692	905.6911	922.1417
970.2006	1040.2194	1072.1507	1095.4224	1111.3809	1148.4883
1175.0674	1184.7434	1211.3073	1259.6126	1278.7417	1317.9535
1338.2983	1378.2631	1388.4151	1417.1762	1438.3919	1443.7566
1444.1271	1448.3729	1457.6431	1458.3995	1463.2944	1801.7221
2955.0754	2960.0771	2970.0545	2977.5622	2986.9150	3000.4191
3012.6784	3032.2084	3036.6547	3042.7441	3069.8946	3102.6854

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Structure   5
===========================

36.1288	68.3588	89.1474	137.9253	176.3725	200.7465
241.3907	253.5662	304.4886	376.2725	497.7936	593.2835
651.7352	730.7477	827.2068	837.6667	871.5393	924.8930
994.0814	1036.6032	1060.7587	1097.6759	1113.2684	1148.6774
1178.0738	1193.5650	1229.4830	1269.2569	1288.0096	1306.8052
1339.4949	1368.6080	1378.9623	1422.0158	1434.2044	1443.0537
1443.8224	1447.2835	1455.1597	1457.7205	1461.2533	1801.3461
2953.5985	2959.2430	2968.6775	2981.1708	2987.0983	2990.0053
3019.6185	3035.8150	3043.4985	3048.5271	3070.2509	3102.6585

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Structure   6
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23.3371	72.5143	89.8839	114.9714	138.9457	186.2837
235.2336	255.1396	303.5781	360.9901	430.9901	637.1246
708.0817	723.5612	776.9836	866.6515	891.0453	916.4148
1015.6831	1045.8740	1058.5812	1101.5080	1109.6788	1148.5191
1177.8919	1194.5365	1230.2243	1263.9921	1289.7361	1302.7301
1328.4426	1370.1124	1378.0206	1428.0331	1437.9219	1443.4660
1445.9614	1453.5397	1454.9944	1457.7367	1464.5189	1802.5363
2951.8857	2959.9499	2962.6675	2979.2016	2987.2593	2987.8769
3016.7041	3036.9593	3043.9592	3054.5888	3070.4693	3102.7964

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32.9854	86.8921	114.8015	140.6820	171.7617	223.5834
267.5062	293.7874	320.6895	383.6760	475.0086	570.0099
668.2863	751.8845	806.1423	850.1962	912.1656	917.1085
967.4818	1039.0998	1064.4205	1082.7968	1109.1732	1148.4580
1173.9733	1190.4154	1222.4426	1246.8553	1273.4033	1334.9080
1347.0214	1376.7274	1382.1064	1416.6710	1437.9763	1439.9796
1443.5917	1446.1556	1456.3086	1457.5576	1468.1151	1799.1446
2952.3163	2959.6223	2971.3053	2978.0826	2987.2160	2997.4605
3023.0890	3030.4604	3033.6915	3048.8827	3070.5923	3103.3154

==========================
Structure   8
==========================

22.9687	50.4414	107.4807	140.1412	165.1621	185.9078
259.9660	291.1979	333.5345	409.0017	461.8820	603.2254
686.7950	740.8572	819.0970	837.2932	882.7138	931.5430
961.3261	1029.0170	1066.2538	1090.4125	1111.2560	1148.3761
1166.4529	1179.7610	1218.5747	1268.3512	1286.8161	1324.5913
1339.6616	1358.1673	1379.5948	1428.1062	1434.3174	1443.5353
1445.4885	1448.8007	1457.3749	1457.7427	1469.3528	1800.1177
2955.3748	2959.6486	2968.9121	2986.7069	2994.7974	3000.2621
3022.1128	3036.4198	3047.8189	3064.7498	3069.6655	3102.7339

==========================
Structure   9
==========================

23.5783	51.5460	109.4585	116.6409	140.2003	207.7136
229.2530	275.5726	294.3105	402.5915	433.9081	627.6231
720.6306	728.6421	771.1416	865.7751	877.2122	931.4716
967.3883	1047.9419	1072.9618	1091.4596	1110.7645	1148.5195
1177.8105	1184.3776	1235.0333	1271.3855	1279.5110	1318.8182
1336.9179	1361.8023	1379.7554	1427.9538	1437.5893	1443.3189
1445.0318	1449.7780	1457.8340	1458.5603	1463.5877	1801.8016
2958.0363	2961.2652	2967.8286	2986.8479	2987.1667	2999.7465
3016.6029	3038.2081	3043.7731	3053.9913	3070.1944	3102.5436

==========================
Structure   10
==========================

23.5001	50.9613	101.1967	124.5887	141.3253	205.9427
230.5068	277.0316	296.1630	413.5228	419.4636	627.5353
707.2961	741.6367	779.8952	869.3776	876.5654	923.4966

```
 969.2756   1042.9926   1075.0351   1095.7293   1108.2018   1148.6274
1177.3940   1183.9991   1239.1060   1258.6123   1291.1131   1318.3049
1337.5177   1362.7545   1379.8160   1428.5284   1438.3309   1443.5473
1444.0856   1450.0963   1457.7866   1458.9534   1463.3250   1801.8291
2956.1958   2960.8272   2962.2753   2978.8654   2987.0709   3000.3329
3021.8944   3038.6337   3044.6020   3066.3503   3070.2209   3102.5426
```

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          ==========================
                Structure   11
          ==========================
```

```
  50.9253     63.1419     97.9178    141.7157    177.7971    211.8418
 259.9607    298.5208    315.8840    392.8030    478.2659    583.2222
 661.3497    753.5054    803.2964    847.5829    878.4845    917.6957
 972.1316   1035.1816   1071.2316   1086.2293   1111.0587   1148.0367
1178.5560   1194.0097   1225.7452   1268.6186   1285.7233   1336.1506
1342.6910   1359.0527   1381.0455   1418.6679   1434.3891   1442.2027
1443.3842   1446.2999   1456.6098   1458.0153   1469.8881   1797.5715
2955.3290   2962.4276   2970.7273   2978.3212   2986.0340   2997.7094
3021.5502   3040.6391   3043.4916   3044.5949   3069.2166   3102.0235
```

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          ==========================
                Structure   12
          ==========================
```

```
  48.3265     74.0559    110.9561    132.9007    195.4003    228.5092
 241.3858    254.8987    281.4739    406.6109    530.4241    548.6960
 584.5919    712.4159    783.4638    832.5547    877.5071    924.4528
1013.2859   1053.3307   1081.4636   1088.3713   1115.9770   1139.8109
1151.2994   1199.7248   1226.6293   1249.7634   1287.4089   1295.1959
1366.1263   1373.8105   1379.4753   1407.6802   1433.8672   1447.5026
1449.2595   1455.5716   1458.2562   1461.3136   1463.3050   1821.5992
2950.5257   2958.6229   2959.7835   2966.8730   2970.3848   3004.8044
3011.4598   3026.0471   3039.1445   3043.9726   3044.3855   3088.6179
```

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          ==========================
                Structure   13
          ==========================
```

```
  35.5626     80.5571     99.4917    108.1027    130.3072    197.5410
 238.2671    245.5484    298.7136    392.9820    528.3451    533.2690
 587.4982    709.5683    785.2610    839.3191    895.6698    910.0537
1027.9077   1066.1698   1083.4746   1090.2509   1114.4366   1138.7301
1149.1146   1196.8396   1209.5240   1267.6100   1275.1518   1287.2379
1344.9100   1377.9587   1388.9289   1410.4846   1442.4480   1446.8005
1450.3917   1454.9931   1458.3030   1461.5754   1464.0213   1823.7780
2946.7533   2956.9288   2961.5880   2967.3268   2981.4298   2981.8896
2996.7388   3029.8776   3039.2214   3043.8453   3044.1524   3088.7826
```

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==========================
        Structure   14
==========================

  31.0274      74.0245      96.6259     118.3186     144.8142     198.5363
 244.1651     271.3694     310.2214     425.4440     503.5315     534.9920
 590.2630     727.1406     780.1155     843.4938     877.6192     922.3728
 979.0101    1070.5545    1085.3624    1093.0635    1111.0093    1139.0194
1148.6516    1184.6388    1213.6680    1258.5296    1283.7839    1313.9890
1337.9866    1378.3087    1385.1528    1410.9724    1442.6170    1445.9255
1447.8393    1457.0576    1459.1107    1462.1219    1463.2443    1823.6606
2954.5726    2957.8141    2960.4015    2967.0785    2982.1258    3000.9235
3003.5323    3034.5819    3036.0270    3042.3310    3043.4369    3088.5757


==========================
        Structure   15
==========================

  46.0186      50.0523     117.2952     142.1049     199.8696     215.4490
 255.0684     262.3307     347.7800     410.1493     525.2304     533.6492
 581.2254     723.7558     785.3292     821.3478     879.7453     929.0097
 974.4113    1057.7289    1075.9690    1084.0414    1117.9928    1139.7073
1151.1668    1182.3170    1218.8431    1245.5532    1284.9139    1328.4702
1357.2774    1373.9220    1379.5715    1409.8110    1431.9847    1447.4519
1449.8340    1457.1478    1459.5929    1462.8776    1464.1291    1821.1462
2956.8134    2962.0787    2966.4252    2972.1420    2976.7675    3014.3237
3015.9592    3032.4973    3037.9289    3041.3727    3044.1459    3088.3161


==========================
        Structure   16
==========================

  45.3419      96.3700     119.0158     135.4008     203.8977     226.5133
 259.2729     297.5134     314.9653     421.1364     527.4831     528.0490
 578.6438     743.7405     774.9678     829.2915     888.5680     920.8431
 978.6432    1065.9909    1084.3378    1084.6123    1108.3260    1139.8116
1149.5001    1198.1288    1220.0039    1245.6809    1272.9565    1335.3858
1346.3152    1375.9736    1383.6189    1407.8208    1436.2985    1443.3573
1447.6267    1454.1450    1458.9736    1461.8517    1464.1626    1822.3988
2947.3577    2960.2815    2963.3498    2966.8990    2979.5065    2996.9358
3007.8792    3033.1748    3035.0888    3044.2526    3056.0678    3088.0535


==========================
        Structure   17
==========================

  50.5702      74.0302     108.6734     121.6780     156.4066     205.2123
```

236.0208	258.1958	329.9553	374.9186	469.3950	583.9233
706.5398	711.3731	771.8654	828.5424	895.2659	914.5243
1008.8494	1055.2479	1059.6571	1099.1369	1121.2216	1141.3261
1160.1320	1192.7948	1224.8547	1256.6874	1285.9062	1297.6052
1328.2991	1366.5493	1378.3858	1442.7199	1443.4075	1447.8509
1453.1178	1455.3103	1461.6508	1463.6079	1469.4400	1820.4312
2952.1348	2959.1153	2961.9313	2967.4953	2988.5971	2999.1602
3013.2967	3038.3578	3045.9945	3046.1379	3057.6372	3087.4234

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==========================
      Structure   18
==========================
```

54.4806	89.4732	123.6233	147.1133	179.4399	198.6029
250.7499	314.4358	338.4389	434.2916	479.5947	564.7278
708.2853	711.6097	777.7917	817.2208	884.1099	931.9221
959.9840	1048.1320	1068.8831	1101.1622	1113.1216	1140.8714
1147.2994	1180.5678	1215.9268	1263.7089	1287.1938	1320.6324
1335.2891	1361.4522	1379.2681	1434.6206	1444.7327	1448.1862
1451.0445	1454.0397	1462.3056	1464.4166	1475.3744	1814.7278
2958.3300	2960.1741	2969.2306	2969.9495	3000.7447	3008.2809
3015.4072	3036.7482	3049.9873	3053.3374	3064.6235	3088.4718

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==========================
      Structure   19
==========================
```

54.0848	65.6707	102.6993	125.9439	195.0152	197.8166
236.7079	248.4686	326.7711	420.5544	471.0777	563.4045
695.5959	727.5727	768.7674	824.7833	876.4405	928.4540
994.9278	1041.7511	1061.9102	1097.9720	1120.4087	1141.2473
1156.7439	1189.6830	1217.2836	1263.5871	1286.3812	1305.5552
1329.3529	1369.9230	1380.7525	1438.8230	1445.9255	1447.6332
1449.0352	1455.8285	1462.5929	1462.7996	1465.7689	1818.1515
2954.2893	2958.2565	2969.1949	2970.7958	2992.6941	3004.9223
3016.5865	3036.9026	3045.4375	3049.2770	3058.3202	3087.9340

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==========================
      Structure   20
==========================
```

36.4431	61.6358	111.1773	138.4987	172.1451	207.2298
227.5173	276.6876	324.5194	417.7556	470.9634	582.2723
695.9409	723.4817	772.3973	828.2123	881.0126	930.0774
960.1409	1064.5443	1072.3513	1086.6505	1120.1343	1140.9294
1156.8692	1184.0697	1227.8501	1264.7487	1273.7979	1318.2877
1335.5628	1357.3789	1378.9812	1439.2748	1444.4946	1446.1094
1451.4943	1457.2252	1462.9635	1464.3598	1467.9063	1820.1673

```
2956.5661      2959.6439      2962.7179      2967.3311      3004.1830      3004.9523
3016.5950      3036.0779      3044.8667      3046.0432      3061.3516      3087.3784


                        ===========================
                             Structure  21
                        ===========================


     43.3676        63.4611       117.0215       134.1621       170.6649       206.0253
    226.2958       281.9710       329.9898       414.3436       471.5077       581.7306
    696.5252       723.2961       774.0382       836.8534       879.7313       921.9008
    962.0394      1059.0080      1072.8834      1089.4776      1121.0864      1141.1555
   1155.9568      1185.2646      1232.0164      1251.1719      1286.0607      1314.9075
   1336.4441      1356.8487      1380.7762      1440.0918      1444.0305      1446.2723
   1451.2543      1458.0705      1463.1689      1464.2595      1468.1797      1820.2558
   2954.8160      2963.5230      2964.3295      2967.6025      2997.5721      2999.5711
   3013.1204      3041.2315      3045.7981      3045.9344      3066.0514      3087.1913


                        ===========================
                             Structure  22
                        ===========================


     50.4838        93.3254       115.7195       131.4071       182.0344       189.8718
    218.6376       308.2678       337.3515       402.6648       472.4773       562.5372
    696.7914       731.1843       764.1471       821.2653       896.7280       933.5535
    966.8761      1052.6564      1076.4336      1078.2165      1119.7737      1140.4217
   1155.7881      1191.1107      1212.3710      1262.9882      1284.4286      1320.2232
   1334.1133      1360.9343      1383.2278      1437.2175      1443.1697      1447.3320
   1449.5506      1458.8420      1461.6533      1462.5601      1464.7352      1815.5139
   2962.3886      2963.4661      2967.8249      2971.8052      2997.4291      3010.4316
   3013.3209      3038.3516      3052.6117      3057.7731      3060.2460      3089.2911


                        ===========================
                             Structure  23
                        ===========================


     39.9811        94.5982       104.8508       153.1063       185.7604       215.7262
    225.5678       278.5287       336.8674       429.5100       454.6442       562.2592
    692.6837       752.2383       771.1656       817.1681       887.9738       932.7987
    962.3776      1059.0515      1077.1864      1081.1197      1120.8006      1141.4955
   1153.1347      1186.5018      1216.2676      1265.5236      1271.4337      1325.2824
   1333.4141      1348.3247      1388.5636      1439.1477      1443.4039      1447.9920
   1450.1083      1460.4251      1462.9026      1463.5460      1465.1442      1821.0896
   2955.4074      2958.4610      2964.1401      2969.5049      2993.6759      2998.8502
   3012.7396      3039.2359      3049.6538      3053.7487      3056.7495      3088.3521
```

S.3.2 $(\mathbf{TS}_{\alpha'})^{\ddagger}$

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        Structure    1
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```

1431.5249i	34.8851	69.5268	84.8107	113.0097	142.2970
210.6833	239.8106	248.5080	301.3207	313.6445	373.0964
510.3671	538.6479	567.4610	646.0675	726.4596	824.3386
827.7190	898.5196	921.0004	1006.1636	1052.3425	1052.7613
1078.9165	1092.6662	1125.0365	1156.9655	1191.2702	1205.6500
1228.7585	1235.5216	1250.7542	1285.9472	1293.3230	1364.5268
1373.7016	1380.1743	1412.4036	1421.9840	1435.6085	1448.9618
1455.4152	1461.4229	1550.7903	1811.4609	2953.1269	2959.0439
2967.9437	2976.8883	3000.5057	3017.2527	3026.3194	3037.3672
3038.2343	3043.6739	3151.5068			

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==========================
        Structure    2
==========================
```

1431.5268i	33.7493	72.1943	89.4916	107.9736	146.7742
210.6110	240.4010	250.0574	300.6392	309.4333	375.3524
511.0758	537.7439	569.3236	645.6709	726.1733	823.6730
828.6720	899.1339	921.2796	1006.3926	1052.3981	1053.9473
1077.5610	1092.4552	1124.7292	1157.0447	1190.2355	1206.3631
1227.7786	1236.2132	1250.7687	1286.2480	1294.2697	1364.7336
1373.8090	1380.4896	1412.4873	1422.0722	1435.7121	1449.0265
1455.4284	1461.4573	1551.7069	1811.0539	2954.4763	2958.7785
2967.5197	2976.4378	3002.7068	3017.6568	3026.4296	3037.6498
3037.7509	3043.7200	3151.2777			

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==========================
        Structure    3
==========================
```

1430.9007i	30.3639	63.9589	90.9246	109.1452	115.2264
146.7794	238.2038	257.0033	294.9809	315.5946	359.8338
479.0737	537.1845	565.7875	690.2768	708.1428	778.3261
877.2820	906.8472	908.0196	1021.4722	1054.5772	1063.6291
1079.8422	1096.1544	1122.1999	1157.3509	1193.3029	1195.4999
1222.6806	1238.6142	1267.3331	1270.5850	1287.0590	1344.1913
1377.8670	1390.3716	1414.5140	1421.8060	1443.9422	1451.0541
1455.0401	1464.2870	1549.8994	1813.8784	2949.5688	2960.9755
2969.6790	2977.3576	2983.8477	3006.7756	3027.3166	3037.6129
3038.2140	3044.0354	3150.7866			

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        Structure    4
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                        =========================

 1431.0118i       31.2695        48.4289        94.4351       114.1235       153.4813
  192.8508       256.1168       276.7505       310.3486       354.6361       391.4194
  476.1201       536.9778       571.2236       649.1167       736.2718       813.5057
  830.8828       898.5188       929.7470       967.7704      1053.5449      1058.8221
 1076.8716      1082.1576      1125.7044      1156.9108      1175.6588      1202.1525
 1223.3509      1231.1654      1249.3981      1281.9845      1328.3762      1355.9948
 1374.1886      1380.1504      1414.9811      1422.2994      1433.9072      1449.7321
 1458.5544      1464.1392      1551.1189      1810.5786      2958.7881      2967.4144
 2972.7321      2980.2103      3011.7025      3021.0136      3035.5306      3037.7038
 3038.4250      3043.1666      3151.3081


                        =========================
                           Structure    5
                        =========================

 1431.6659i       32.5196        49.2988        87.7511       123.3751       148.6386
  194.4413       257.1722       275.8291       315.0464       352.3871       392.3908
  475.7674       538.1790       568.9008       649.4099       736.4881       814.0489
  830.2848       897.3441       930.2267       967.9288      1052.0294      1059.1290
 1077.2176      1083.2870      1126.0738      1156.6595      1176.9811      1201.9153
 1224.0807      1231.3198      1249.4357      1282.0237      1328.1985      1356.1311
 1374.2297      1380.1641      1415.0562      1422.1951      1434.1497      1449.7162
 1458.6908      1464.1964      1550.3875      1810.9938      2958.8092      2968.0309
 2972.8163      2981.0381      3011.4589      3021.4156      3035.3770      3038.0903
 3038.3373      3042.5708      3151.5102


                        =========================
                           Structure    6
                        =========================

 1430.9151i       27.8393        55.8723        93.9328       105.6502       138.1564
  146.0713       233.6327       274.7718       309.2344       325.8870       412.9330
  437.7011       537.3160       566.9450       687.2268       731.7496       775.1924
  866.5068       900.0771       921.1845       973.1745      1055.0143      1071.3339
 1083.5091      1094.7131      1116.4185      1157.4075      1184.8178      1195.1189
 1224.4865      1239.8684      1258.3644      1278.4175      1313.0020      1338.2636
 1378.5388      1386.8714      1415.4602      1421.1590      1444.0191      1447.8275
 1457.9746      1463.2737      1549.7452      1813.4646      2956.3769      2960.3175
 2970.1832      2977.8884      3001.7103      3012.2847      3032.2679      3036.9046
 3037.5640      3043.3314      3150.7235


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                           Structure    7
                        =========================

 1431.0680i       28.4487        55.7449        92.3355       107.4764       139.8521
```

```
  144.8092      234.9267      272.1082      310.4186      326.9928      412.5175
  437.9700      537.2537      566.9952      688.0518      730.9937      775.1661
  866.8229      900.6762      920.8102      973.3979     1054.8128     1071.3187
 1083.1341     1094.5176     1117.3199     1157.5404     1184.6667     1195.0954
 1224.4257     1239.8143     1258.4793     1278.7302     1313.1143     1338.2291
 1378.8411     1386.9225     1415.4005     1421.3211     1444.0628     1447.8900
 1458.0865     1463.5068     1549.8510     1813.5068     2955.8782     2960.6649
 2970.3679     2978.2742     3001.5704     3012.0042     3031.9758     3037.3450
 3037.5254     3043.3942     3150.7103
```

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                     ===========================
                         Structure    8
                     ===========================
```

```
 1429.0904i      34.1254       61.3769       85.9926       99.7548      146.6445
  199.9248      241.0437      254.0302      309.4693      322.7501      388.3257
  490.3570      534.8365      604.7363      656.8177      732.6735      823.9537
  831.0430      868.9823      924.9618      994.0769     1041.8224     1061.1379
 1074.6166     1101.8741     1136.9180     1161.0582     1191.1357     1211.7952
 1227.6181     1233.6292     1262.7169     1288.9241     1304.2455     1334.9783
 1368.6325     1379.8562     1418.2729     1423.1797     1441.6997     1447.2553
 1455.3750     1461.3401     1547.7002     1813.2670     2952.5002     2959.6079
 2970.2375     2982.5899     2989.3243     3020.1820     3035.8762     3038.3432
 3045.0103     3052.3147     3151.5755
```

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                     ===========================
                         Structure    9
                     ===========================
```

```
 1432.2833i      33.9384       66.6577       86.4909       99.9780      148.0060
  200.5609      241.5486      252.3750      301.7979      331.6122      390.6342
  492.1122      536.6200      597.4459      655.5201      731.9478      825.5275
  830.7781      867.4800      924.0616      994.7627     1041.7754     1059.0069
 1075.3813     1101.8364     1136.2945     1160.9439     1191.4303     1213.3935
 1228.6693     1234.1844     1263.1776     1288.3264     1302.9185     1336.3551
 1368.7205     1379.4841     1418.2897     1422.0149     1441.7210     1447.4131
 1455.3560     1461.4712     1550.7720     1812.7989     2953.1456     2959.9262
 2970.4034     2982.1538     2989.5397     3020.5713     3036.4591     3037.4588
 3044.6451     3051.0328     3150.5571
```

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                     ===========================
                         Structure   10
                     ===========================
```

```
 1432.1569i      25.7953       72.2133       73.6135      105.8514      115.0572
  160.5019      235.7281      257.9426      309.6823      321.3138      367.2547
  433.6755      537.0090      645.0612      710.7047      726.4323      774.1053
  856.4201      891.7368      916.6608     1013.4140     1052.8385     1057.5374
```

1072.3182	1100.8488	1137.5207	1161.5492	1191.8167	1214.2724
1226.9566	1239.3237	1261.6596	1288.3424	1296.6293	1323.7725
1369.2309	1378.3173	1417.8418	1430.6507	1446.0256	1453.5581
1455.1292	1464.4869	1548.1014	1813.7169	2952.7869	2960.8953
2965.3829	2983.3537	2988.5961	3017.4120	3037.7606	3038.0878
3044.7853	3058.0974	3150.8445			

==========================
Structure 11
==========================

1432.2519i	25.5401	69.7739	85.2478	101.2396	115.1502
160.6202	235.9169	252.4306	298.3039	337.9104	371.0057
431.8466	537.7473	637.7784	709.5997	724.9124	775.1547
855.8388	891.5649	915.5206	1015.2572	1053.7136	1058.0111
1072.3958	1101.2075	1137.4169	1161.6821	1192.0152	1213.9863
1227.5966	1238.8048	1261.5593	1288.4338	1296.6996	1324.0507
1369.7382	1378.3316	1418.2673	1429.2736	1445.9961	1453.4408
1455.1724	1464.4533	1549.6785	1813.6398	2952.8907	2960.5245
2963.7446	2981.5214	2988.8992	3017.0356	3037.6209	3037.6775
3044.8441	3057.1094	3150.8217			

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Structure 12
==========================

1427.5244i	37.2301	84.6476	105.8387	113.6786	153.2514
225.2246	263.6984	291.5523	317.5126	329.2653	396.2793
475.0165	535.1376	576.2169	668.6768	750.6132	804.2571
844.7624	908.4030	915.2978	969.1061	1057.8716	1063.2355
1077.8081	1082.8384	1119.0793	1155.6127	1184.4183	1204.6018
1222.9772	1231.0573	1247.3040	1272.4269	1334.6237	1345.3129
1373.2162	1381.9731	1414.9411	1423.4225	1438.4333	1445.1368
1454.6128	1466.5297	1553.5786	1810.4117	2952.9997	2960.4875
2971.3571	2978.6760	2998.2074	3024.5290	3032.5666	3034.4263
3038.6153	3049.4546	3152.4891			

==========================
Structure 13
==========================

1427.8944i	28.7546	64.1911	92.0000	116.6337	158.9731
172.2102	258.8811	294.7657	326.6955	337.5307	414.9790
461.7589	535.1346	612.5849	687.3812	740.3829	817.1971
828.7644	880.1793	931.8839	960.4293	1038.8407	1063.5362
1073.4945	1100.4539	1128.5516	1156.3868	1173.2961	1210.7385
1218.0907	1233.3344	1265.0156	1281.7265	1321.0910	1339.3293
1357.0420	1380.8566	1418.3064	1428.3074	1443.6107	1449.3495

1458.2232	1469.6008	1547.5165	1811.1345	2954.6058	2960.0226
2970.3634	2996.0140	3001.1595	3023.0365	3036.8857	3038.2810
3048.8104	3067.1062	3151.7004			

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==========================
        Structure   14
==========================
```

1431.3228i	31.4370	78.8709	96.1162	124.7886	145.0715
220.0717	262.4373	299.0966	316.9457	325.2191	394.1448
478.8721	537.4305	564.7295	667.2217	750.4403	803.6756
845.6300	907.4592	915.5679	970.6441	1053.9001	1064.0036
1079.7726	1083.3138	1119.5388	1156.1538	1187.0192	1204.5783
1225.2378	1232.0906	1248.7387	1272.3267	1334.8993	1345.8007
1374.9302	1381.6277	1414.0327	1422.0815	1438.1330	1445.8816
1456.2043	1465.1113	1551.6163	1810.8989	2953.1551	2960.2634
2971.4761	2978.9165	2998.8139	3023.3787	3030.4843	3034.3610
3038.4353	3049.6157	3151.7366			

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==========================
        Structure   15
==========================
```

1432.9750i	24.6063	48.8863	92.2111	109.3230	159.4467
170.6496	257.5302	302.7119	305.9125	354.4659	415.4230
461.8826	536.8956	606.1310	684.6698	740.4360	817.8469
829.7840	878.2656	931.4282	961.4936	1038.3842	1061.9073
1072.6707	1099.8097	1129.3655	1157.4905	1173.2107	1214.3801
1218.3943	1234.6885	1265.3847	1282.2658	1321.2829	1340.6217
1356.4872	1380.3245	1418.5504	1428.1984	1443.2049	1448.7585
1457.6523	1469.2097	1549.7596	1811.2756	2955.6406	2960.1087
2970.4844	2995.3018	3001.2147	3022.9543	3037.0663	3037.2165
3047.2232	3066.6485	3150.4618			

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==========================
        Structure   16
==========================
```

1431.6351i	25.0964	49.3646	82.7043	111.4783	116.3340
187.3885	228.8462	276.1138	307.3191	319.7150	407.8613
435.8760	536.8493	635.8440	725.6086	728.1853	769.4352
855.2461	877.4871	931.6419	964.6941	1054.9715	1072.0320
1074.6649	1090.2210	1136.4773	1161.0598	1183.4569	1213.2288
1228.9582	1240.5975	1266.5489	1279.1535	1309.4004	1337.0593
1360.3055	1380.1701	1417.7863	1430.4083	1444.9622	1450.1176
1458.6554	1463.5484	1548.0835	1813.3859	2959.4913	2961.6077
2969.1135	2990.7956	3001.5121	3017.5087	3037.7137	3038.5802
3044.3513	3057.9084	3150.7570			

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                            ==========================
                                 Structure  17
                            ==========================

   1432.1011i       25.8975       48.7952       95.9118      106.7230      115.1807
    185.9799      225.2669      275.3079      296.9453      338.4578      408.1443
    434.6766      537.9141      628.4991      724.4680      727.7382      769.9624
    854.8423      877.2172      930.6352      966.3463     1055.3065     1071.9095
   1075.0593     1090.8938     1136.7899     1161.6145     1183.4014     1212.9720
   1229.9482     1240.1397     1266.5268     1279.6803     1308.7140     1337.1237
   1360.7619     1380.3522     1418.2184     1429.2397     1445.0280     1449.8781
   1458.6815     1463.7161     1549.3759     1813.2378     2959.1568     2961.8200
   2967.9825     2989.2335     3001.0238     3016.6281     3037.5519     3038.8175
   3044.6350     3056.6923     3150.6305


                            ==========================
                                 Structure  18
                            ==========================

   1431.9554i       26.1023       49.8141       79.1762      109.9327      120.8481
    187.3772      229.3346      275.7551      309.5170      321.9124      413.6178
    426.8371      536.8792      635.7873      711.7662      740.5608      777.4270
    860.8477      876.0956      923.5034      966.5712     1050.8999     1068.9431
   1077.2922     1093.5530     1135.5288     1160.9677     1181.7409     1215.2809
   1231.5861     1241.8018     1256.1278     1290.0157     1307.4213     1337.2384
   1361.0383     1380.3092     1417.8629     1431.2398     1444.0904     1450.1725
   1458.8317     1463.3586     1547.2790     1813.3243     2957.5235     2962.4515
   2964.4956     2983.6353     3001.7340     3021.1904     3037.7727     3039.3303
   3044.9893     3068.6897     3150.8018


                            ==========================
                                 Structure  19
                            ==========================

   1425.5278i       57.9985       69.2374      103.0754      115.9369      169.8179
    211.8026      265.3057      305.7872      319.6171      334.5259      398.8154
    479.6743      535.6088      589.8674      659.6546      753.1857      801.9931
    837.7880      875.8766      915.4170      971.8735     1043.8503     1059.6625
   1078.0173     1091.6366     1135.8632     1159.3554     1193.1368     1212.0692
   1224.4961     1235.6577     1264.1580     1277.6192     1336.0717     1339.3709
   1359.1767     1381.5685     1417.4430     1418.9648     1440.6120     1445.4862
   1457.1244     1468.7548     1551.1787     1808.5132     2955.6809     2964.1150
   2970.3779     2977.9495     2998.4080     3022.0932     3037.7227     3042.2897
   3045.2478     3046.8897     3151.1217


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                                 Structure  20
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  1431.0998i      50.4981       60.1309       93.8985      103.9398      153.6099
   207.7888      263.6193      295.1582      312.3590      342.5997      399.7306
   477.4255      535.4389      584.6498      662.9195      753.7103      802.0610
   839.6408      875.5259      915.3936      971.8112     1043.7266     1061.4655
  1078.5087     1091.8145     1135.7790     1160.8272     1192.9594     1212.6308
  1224.9337     1234.7455     1265.6851     1278.2249     1336.3676     1339.4610
  1359.0331     1381.8786     1417.1827     1419.1549     1440.9016     1446.3711
  1457.6496     1471.2465     1551.7307     1808.6010     2956.6281     2962.5608
  2971.5089     2978.7054     2999.1847     3022.5643     3037.2960     3041.1369
  3044.1205     3045.5664     3150.4328


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                          Structure  21
                        ==========================

  1445.0128i      52.3261       74.4083       96.8476      129.0213      187.9027
   230.7997      242.4960      259.9022      280.0399      313.3010      411.0211
   527.7504      531.4600      572.0279      584.7957      712.7747      784.7859
   832.7408      879.3272      924.9239     1013.4520     1053.8890     1068.5677
  1083.0505     1090.0302     1126.5866     1161.3476     1198.5727     1219.4851
  1237.0348     1242.3435     1263.9459     1289.1131     1296.0624     1365.0338
  1373.0460     1380.1852     1410.8501     1434.7332     1448.2965     1449.3062
  1455.6489     1461.4423     1498.4503     1833.0281     2954.5364     2959.0635
  2959.7397     2971.7891     3006.7710     3013.8642     3014.7665     3026.8556
  3039.1039     3044.7288     3127.6692


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                          Structure  22
                        ==========================

  1445.5392i      58.4500       77.0305      101.9177      107.2764      140.1288
   186.9924      238.1905      249.7961      297.3229      311.4701      397.8121
   508.7279      537.0988      560.9854      591.4433      710.4844      786.0105
   841.0850      896.6852      910.8001     1027.5727     1065.5016     1068.0835
  1084.7658     1092.2621     1122.0675     1160.6127     1197.2891     1207.0007
  1242.3816     1243.9911     1269.6124     1278.1035     1289.3379     1343.1527
  1378.2218     1387.7660     1413.4847     1443.2444     1447.5270     1451.0576
  1455.1230     1464.1262     1497.4505     1835.0571     2948.2703     2955.4498
  2961.9222     2981.0706     2983.4840     3003.5861     3014.9631     3030.5727
  3039.6045     3045.0166     3127.5236


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                          Structure  23
                        ==========================

  1442.8857i      47.4584       72.1785       87.7883      123.6643      185.0745
```

232.7590	242.0057	247.8989	277.6042	316.0398	413.4728
510.9264	536.3130	569.5182	589.2522	711.6578	784.6495
832.3854	877.2577	923.9221	1015.5848	1054.2489	1065.6932
1082.4532	1089.2037	1126.0988	1158.4408	1200.2396	1211.9047
1242.1194	1243.1916	1260.0577	1288.1486	1294.7938	1365.8106
1371.5969	1379.0831	1408.4922	1435.1083	1447.7196	1449.4683
1455.6006	1461.4328	1501.6129	1833.3206	2950.8728	2958.9619
2962.1621	2969.4426	3007.4696	3011.5593	3016.5254	3024.7152
3039.0212	3044.5238	3127.8488			

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==========================
       Structure   24
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```

1440.2771i	49.7938	53.8543	103.9288	145.6645	192.2800
218.6909	261.4298	267.7222	312.1011	350.3263	415.5844
514.0741	534.0832	566.2541	583.1340	724.4305	787.5572
821.0810	881.4247	929.8938	974.0812	1058.9119	1070.7955
1076.6690	1086.2228	1127.7082	1161.4924	1183.9538	1213.9815
1229.7668	1240.6890	1261.7725	1284.1762	1328.2835	1356.4668
1373.4804	1380.4941	1413.4361	1432.8421	1447.7963	1450.1646
1458.6007	1465.3535	1496.4202	1832.3408	2956.5788	2961.6122
2972.0160	2976.4558	3014.2963	3014.5318	3022.8923	3036.5084
3037.5249	3042.1992	3127.7097			

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==========================
       Structure   25
==========================
```

1444.7614i	43.3549	78.1192	102.3414	121.1947	142.7535
191.8763	243.6833	270.5812	301.4094	327.4600	425.7361
492.3064	535.1278	558.2205	593.6375	727.8419	781.2448
844.9908	878.8201	922.8196	978.7424	1066.8550	1071.8463
1088.0181	1094.5650	1116.4638	1161.0072	1186.2698	1208.9255
1242.7596	1248.6080	1260.1802	1286.5749	1311.3692	1338.4157
1379.4232	1384.1298	1414.0613	1443.2113	1446.3888	1449.0623
1458.0148	1463.2544	1496.8454	1835.0228	2953.9021	2954.9653
2961.0143	2980.7179	3002.4461	3012.6195	3014.7537	3036.4859
3037.3461	3043.5387	3127.3643			

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==========================
       Structure   26
==========================
```

1444.2776i	42.9740	82.7937	101.1376	116.7991	147.7942
190.4375	244.5876	271.5455	298.2394	327.4438	426.3147
490.7541	537.5026	557.2233	593.8521	728.2230	780.4369
844.8942	879.1049	923.3586	978.7289	1067.0103	1071.4952

```
1087.2077    1094.8868    1117.2154    1160.6530    1185.6848    1208.9792
1242.6493    1245.2589    1264.5652    1287.4916    1311.2502    1338.0075
1378.6601    1383.7168    1414.1617    1443.0795    1446.2907    1448.5979
1457.9120    1463.3695    1497.5686    1834.6675    2957.0307    2959.2939
2963.2016    2982.6102    3002.6671    3005.3278    3014.7600    3034.0364
3036.3202    3043.1922    3127.3661
```

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Structure   27
===========================

```
1443.4203i     46.7458     47.1280     90.9657    137.7836    184.9237
 217.6397    246.4384    268.0288    312.8503    350.9908    415.2111
 501.3107    529.8226    562.9045    585.6565    724.9427    786.1044
 821.3156    880.1045    927.3501    975.6011   1057.9494   1066.7186
1078.0069   1086.1032   1127.3651   1158.5517   1182.7330   1210.2027
1233.9565   1241.9669   1259.5548   1287.6948   1327.5620   1357.7813
1371.9049   1378.9640   1410.5780   1433.0415   1448.0461   1449.8985
1458.5314   1463.6488   1500.9853   1832.7471   2957.3813   2966.8375
2974.1809   2978.4340   3012.8110   3016.8119   3016.8529   3029.7069
3039.1527   3042.1040   3127.5262
```

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Structure   28
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```
1441.1455i     43.7131     86.2369    117.9154    123.7435    196.3160
 228.3799    265.3782    290.3561    315.0280    319.4105    426.3611
 513.4063    528.7601    564.0201    584.5176    743.4689    778.0420
 828.9441    890.4520    921.1228    977.6765   1066.2989   1072.2962
1085.2259   1087.3566   1115.7981   1161.2458   1197.4134   1215.4072
1231.0045   1239.7106   1262.8568   1272.9039   1334.8608   1344.6709
1375.3238   1384.4660   1411.0287   1437.7034   1444.2161   1447.4980
1455.4433   1464.3137   1497.6456   1833.8563   2950.8067   2959.5093
2961.2967   2981.6866   2998.7111   3013.8078   3016.8281   3033.2923
3035.6788   3054.2904   3127.4099
```

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Structure   29
===========================

```
1442.2906i     50.7156     73.3114     93.1633    120.6264    151.2308
 181.4410    235.8501    258.5275    297.7616    347.9028    375.2677
 464.6492    547.7671    591.6688    701.1450    711.8553    771.9129
 826.8581    894.8709    915.2380   1008.0810   1054.1567   1057.1792
1072.3399   1099.4896   1148.5586   1162.4779   1192.8840   1222.2998
1239.5579   1245.3923   1260.3779   1285.1095   1296.5921   1324.4246
1367.0855   1378.7788   1437.9705   1445.4406   1454.6196   1455.5888
```

```
1457.2975    1465.5235    1500.2203    1831.2309    2952.7082    2959.0043
2962.1870    2989.8636    3003.4260    3013.0948    3015.7098    3038.7028
3046.8935    3060.6867    3127.4736
```

=========================
Structure   30
=========================

```
1443.1158i     40.7934      80.9820     110.5590     123.5514     184.2864
 223.0936     256.6910     296.9224     312.8836     321.7188     428.0233
 501.2087     529.6674     561.8245     575.3515     744.2839     775.8258
 830.5575     888.5166     921.7800     978.9784    1065.3893    1068.9754
1085.2559    1087.3868    1113.8565    1157.9976    1199.5250    1209.9086
1237.4901    1242.4221    1257.2649    1274.3459    1335.1873    1346.3980
1373.1154    1384.7611    1407.1689    1436.3439    1443.6108    1448.4628
1455.0137    1460.6587    1501.7973    1834.9546    2947.7861    2962.3531
2964.9358    2980.1957    2998.0257    3009.7038    3016.5331    3033.3817
3036.6127    3056.6648    3127.2392
```

=========================
Structure   31
=========================

```
1441.3157i     53.2939      87.9065     105.4456     142.9977     172.0348
 182.3185     250.5417     296.5853     317.6785     354.4577     433.9182
 474.8185     541.4969     577.3510     704.3494     710.9911     776.6026
 816.3890     882.8625     931.4199     960.4579    1046.0119    1067.9778
1072.9898    1101.1673    1125.1251    1161.9015    1182.9400    1215.6396
1233.8491    1245.3526    1265.7842    1285.3633    1318.1759    1335.6232
1360.2355    1379.8914    1437.9536    1443.0814    1445.5012    1454.7320
1457.1887    1474.2628    1501.9382    1825.3760    2959.0800    2961.0779
2969.7181    3001.3036    3010.4186    3017.5372    3020.0484    3037.6522
3053.0941    3067.6738    3129.4547
```

=========================
Structure   32
=========================

```
1440.6338i     53.2996      65.9922      99.6029     108.3462     175.2573
 195.4111     236.5754     248.4307     297.2377     349.6214     419.2359
 467.2133     541.3361     576.6640     694.3714     724.4131     767.7877
 824.4528     875.3860     928.9811     995.2620    1039.5250    1060.8501
1072.7135    1098.5949    1144.4677    1162.4279    1190.7040    1216.8602
1234.6661    1245.9653    1265.8612    1286.8109    1304.7706    1327.7098
1369.9037    1380.9626    1441.4051    1443.2625    1448.3994    1455.7977
1455.9811    1463.3631    1500.0183    1828.8517    2954.4110    2958.9607
2970.6659    2994.0208    3008.2440    3017.1777    3019.7295    3037.1925
3046.4184    3062.2374    3129.0737
```

```
==========================
       Structure   33
==========================


1424.1836i      20.8965       71.9649       93.3086      123.0423      136.8922
 198.6354      236.1941      263.6900      300.2134      336.5078      390.5161
 465.2592      550.3106      592.5403      694.0691      712.1507      771.2932
 827.5307      896.8301      914.1119     1009.7024     1056.1347     1061.3842
1071.0708     1100.2500     1142.2743     1160.7217     1195.3393     1219.8404
1237.7559     1247.3667     1258.8235     1282.7455     1295.6847     1329.3240
1366.8533     1378.1174     1443.8499     1445.4008     1447.5963     1455.0656
1455.2340     1464.1632     1511.4249     1829.1646     2951.6108     2961.7851
2965.4598     2988.4125     3002.3902     3009.2106     3019.7001     3039.4081
3045.6037     3062.7762     3124.4495


==========================
       Structure   34
==========================


1441.3353i      33.8100       63.0131       95.2917      134.4007      167.6378
 187.6571      227.9017      277.8975      296.2793      345.0406      418.1471
 466.5409      546.7776      590.4041      691.1838      724.1436      772.1733
 826.2971      880.7191      930.8276      959.7121     1061.5776     1071.5342
1073.0834     1087.0166     1143.6781     1162.3578     1185.2857     1222.7459
1242.2933     1245.4836     1265.6804     1274.3057     1312.3497     1335.5571
1357.7689     1380.1123     1436.2106     1444.2899     1451.0634     1458.4977
1461.3525     1463.3156     1499.7910     1831.0758     2955.6644     2960.2238
2963.3386     3005.0984     3008.7427     3014.7710     3016.7214     3036.8189
3046.2325     3065.9728     3127.3394


==========================
       Structure   35
==========================


1442.3655i      42.0735       62.6441      104.6598      125.8920      167.2767
 184.8962      226.7674      281.3699      297.6214      348.7734      414.3843
 466.1267      547.9224      589.4678      691.8976      723.4553      773.9649
 835.2447      879.0510      922.0610      961.8324     1056.0205     1071.6685
1072.8400     1089.8947     1143.6269     1162.5190     1186.2229     1226.7339
1239.2229     1246.3397     1258.2162     1286.4227     1307.4977     1336.9131
1357.0424     1381.3019     1436.3926     1444.4003     1451.1751     1458.4596
1460.8131     1463.8090     1499.7811     1831.0340     2956.2743     2963.6476
2964.4262     3000.1105     3003.4855     3012.7239     3015.6873     3041.6060
3046.9069     3068.4273     3127.2050


==========================
       Structure   36
```

```
                         ========================
   1448.8498i      30.5068        96.3788       104.9308       141.0089       179.3994
    211.8075      250.7734       318.2254       331.1104       345.0517       436.8703
    465.2952      547.6853       563.9288       696.5561       711.7830       772.5761
    815.3035      880.4751       932.3727       959.3540      1045.1432      1062.2271
   1073.6033     1103.3391      1126.2777      1160.9344      1192.3536      1214.6725
   1239.6562     1242.5702      1273.6821      1291.2976      1316.9400      1338.5389
   1357.1105     1381.3918      1432.3412      1446.2162      1446.8819      1458.3168
   1459.5651     1472.7446      1489.6666      1822.0398      2958.0965      2960.9692
   2972.9309     2992.1388      3004.0412      3021.8543      3026.9194      3037.5383
   3053.0123     3062.8973      3126.1730

                         ========================
                              Structure  37
                         ========================

   1448.3625i      39.4833        85.9570        99.5454       124.6681       208.1416
    225.2328      250.6715       266.6523       324.4501       334.6121       416.3051
    467.4657      551.2259       566.1767       686.5017       720.4720       759.8270
    823.5202      876.3975       926.0086       993.7358      1042.7462      1058.4317
   1072.3953     1103.6302      1147.2434      1162.5152      1198.9734      1222.0629
   1240.7040     1242.4030      1276.4111      1291.2691      1310.7302      1324.6669
   1369.2894     1381.4368      1431.0839      1443.3296      1451.1115      1455.4942
   1457.8728     1463.8489      1484.7014      1825.9391      2955.7997      2958.9260
   2975.4918     2985.8698      2995.1582      3019.5898      3022.5329      3035.3647
   3047.0970     3059.3730      3124.7337

                         ========================
                              Structure  38
                         ========================

   1454.3928i      58.3701        66.0296        93.6030       119.6545       139.2989
    190.6354      235.0781       258.1327       321.6209       350.6773       367.5865
    459.0727      545.8802       582.3382       695.4756       710.3885       770.1219
    822.1006      894.6617       915.0993      1010.5777      1052.1161      1055.6385
   1067.8523     1099.5622      1150.5859      1160.2775      1198.1439      1227.7967
   1244.1341     1246.4761      1266.8434      1291.7999      1303.2164      1321.7260
   1369.4740     1379.1299      1431.9341      1445.5968      1453.2625      1455.3331
   1461.3183     1465.9960      1487.2677      1826.7748      2952.8832      2962.3587
   2972.2542     2987.2508      2989.6493      3021.1319      3022.6753      3039.7281
   3046.6107     3056.6477      3125.6994

                         ========================
                              Structure  39
                         ========================

   1424.2308i      44.3739        80.8877        98.4331       144.5150       180.4815
```

190.6727	247.8238	301.2987	326.7391	360.8890	433.9957
471.4941	545.8705	580.6406	707.2572	711.3210	775.5787
817.0190	882.4637	928.8843	958.7791	1047.7985	1057.6719
1072.3830	1101.1461	1123.4851	1158.9613	1182.7245	1215.5082
1235.0217	1255.7261	1265.8124	1284.5594	1316.8549	1333.7415
1362.3678	1378.4817	1437.4132	1444.9267	1446.2839	1452.4347
1455.3420	1473.0227	1512.7468	1825.7565	2958.0879	2965.7117
2972.0058	3006.2970	3008.2527	3012.8148	3022.7258	3036.9225
3051.5154	3067.1914	3123.1642			

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Structure 40
==========================

1426.6394i	40.7876	62.3184	99.3211	103.7139	182.1280
195.1884	236.0320	248.7335	304.1610	360.0571	419.7760
464.5366	545.5903	580.0319	699.2079	727.2714	767.1748
824.1130	874.2189	926.9853	994.4532	1040.0580	1054.8156
1065.3760	1097.5115	1142.4725	1160.4455	1190.6843	1215.5627
1236.4300	1258.1431	1266.7993	1284.9086	1302.3277	1325.3680
1369.5775	1380.1010	1441.1689	1445.2193	1449.4710	1451.1453
1455.6914	1463.9747	1510.7013	1829.4235	2958.3911	2961.2744
2969.2017	2998.8480	3005.6470	3010.8308	3020.5893	3039.0320
3045.3303	3063.6359	3122.3772			

==========================
Structure 41
==========================

1454.4841i	40.5374	70.6904	94.5282	119.9962	165.4848
190.6479	226.7636	278.8558	321.8122	347.8950	413.2107
459.6541	545.5131	578.0471	686.3607	720.7845	772.7767
830.7724	878.2602	921.7451	964.7448	1052.3146	1066.3032
1074.0894	1090.4882	1143.9790	1159.9890	1192.6653	1234.6380
1244.0605	1244.5230	1268.5377	1290.3044	1308.8549	1339.5971
1359.7528	1381.8389	1431.3270	1443.9121	1449.4537	1458.8417
1463.6138	1465.1672	1485.8077	1826.5710	2955.9329	2963.9708
2972.3175	2986.2006	3003.1775	3023.1164	3025.3933	3041.1766
3046.3124	3067.6630	3125.6520			

==========================
Structure 42
==========================

1442.2591i	46.9620	85.1585	101.4338	130.7531	169.3146
186.0967	217.1559	290.3829	325.1504	346.7501	402.1992
466.9313	537.6409	575.2194	692.7587	730.0795	762.2063
820.8550	894.5054	933.0753	966.9491	1049.6688	1070.4498

```
1077.4892    1077.9753    1141.5794    1161.2656    1192.5100    1212.1905
1237.1043    1244.5853    1263.5645    1281.4651    1320.9194    1332.8472
1359.8654    1383.0289    1439.3690    1441.4261    1447.2773    1452.2898
1459.3453    1462.3915    1501.3427    1826.2802    2963.0134    2964.4091
2968.6028    3001.1918    3011.0839    3015.7773    3023.8958    3039.6811
3059.4456    3060.9481    3131.4350
```

===========================
Structure   43
===========================

```
1445.2133i     39.6166      94.0556      97.2543     134.6149     165.8798
 214.8292     227.0418     277.0872     310.2306     346.3362     430.9259
 451.0911     538.9495     573.9450     688.7741     752.6084     769.7534
 815.1332     886.8881     932.8776     962.4059    1056.4884    1073.0050
1078.0115    1079.9139    1142.4835    1162.3376    1188.1956    1216.5847
1232.8919    1248.1403    1267.6547    1271.6549    1324.2850    1332.9878
1349.2418    1388.3277    1440.4037    1443.5229    1449.3455    1451.9516
1462.8098    1463.1207    1494.7143    1831.6506    2956.7555    2958.0203
2964.4119    2997.7150    3000.6966    3013.6090    3022.3535    3039.8235
3056.6574    3057.2732    3129.8396
```

===========================
Structure   44
===========================

```
1447.5740i     52.5075      71.4775     104.0190     131.3872     179.1701
 195.8982     221.6319     319.4147     335.2496     349.3765     408.2578
 463.2520     541.5752     562.1848     684.1538     730.1328     759.5509
 818.4700     892.0873     928.6281     968.6139    1047.8767    1057.9004
1074.2590    1080.4859    1143.5141    1159.1068    1198.2013    1214.1138
1240.7472    1246.9193    1268.9807    1291.4296    1325.5730    1334.7357
1359.1071    1385.0536    1432.3288    1442.0114    1449.9976    1456.0981
1461.0880    1462.8386    1495.5044    1823.4112    2963.9487    2967.8335
2974.1439    2990.0097    3007.2957    3019.0791    3023.4253    3042.6354
3056.2943    3056.9853    3126.0401
```

===========================
Structure   45
===========================

```
1426.1082i     42.1833      67.7873      97.6731     130.8057     167.9358
 185.6836     212.7996     294.1435     338.0287     364.6335     398.7783
 463.4064     545.1845     580.3265     700.0757     726.0080     763.1531
 819.7225     895.8297     934.2374     966.5407    1045.7347    1055.9920
1077.4621    1080.1328    1140.7478    1159.1371    1191.2675    1211.1690
1239.4936    1259.5815    1266.4400    1279.7845    1316.6529    1331.7694
1360.3188    1382.1391    1439.1343    1443.2210    1449.4868    1450.5336
```

1458.9771	1460.8610	1515.0586	1827.8778	2965.0362	2967.3332
2973.7959	3001.5318	3006.8026	3010.4456	3021.6563	3039.8650
3059.6956	3060.4278	3122.6345			

```
===========================
      Structure   46
===========================
```

1436.0213i	30.1086	81.7569	90.9805	115.5734	179.4596
221.0890	223.4554	275.1404	326.4228	371.5490	434.0150
449.4729	547.7060	578.1596	694.4925	750.4111	766.5255
811.1886	883.4568	929.7329	960.8000	1042.2609	1057.3709
1078.4902	1081.7745	1142.3896	1160.3378	1187.9079	1213.7905
1237.3087	1264.9481	1269.7154	1279.4035	1319.7860	1334.1927
1349.8732	1387.3234	1437.9408	1442.3533	1446.7642	1449.9894
1460.1667	1463.4970	1507.1998	1834.8023	2954.5385	2964.5222
2969.5197	2997.4531	2998.9944	3002.6822	3022.8381	3038.7840
3055.1281	3058.5438	3120.1683			

S.3.3 $(\mathbf{TS}_\alpha)^\ddagger$

```
===========================
      Structure    1
===========================
```

1439.7402i	49.0526	72.0542	87.4168	134.1456	163.8489
187.1222	212.0895	238.5742	283.0977	295.8508	334.6258
397.0623	509.1733	641.9796	680.1567	729.0732	831.9210
849.1406	901.6377	928.7807	1006.8644	1039.3983	1051.9817
1071.7159	1113.9065	1146.8967	1159.8192	1173.5804	1211.8933
1228.2944	1245.6476	1269.2008	1289.7171	1339.4728	1372.1432
1375.0631	1386.7692	1432.4764	1440.6750	1442.1853	1447.0282
1453.2607	1456.1171	1459.1628	1776.9752	2955.0747	2957.0433
2967.8685	2984.1746	2999.9482	3022.3078	3036.1628	3041.3895
3053.3433	3067.2190	3101.0593			

```
===========================
      Structure    2
===========================
```

1445.1558i	49.3366	65.1183	95.8974	113.7884	135.5488
170.3706	236.1988	244.3815	297.9026	311.2737	327.2940
336.4667	486.6713	677.7871	701.6567	711.3470	802.2679
881.4943	905.4977	922.7067	1012.4330	1045.9767	1059.7838
1074.0215	1114.6595	1147.0237	1165.0808	1172.6179	1200.8894
1228.0001	1228.4208	1268.2255	1279.3192	1345.9570	1360.9372
1377.1076	1394.4018	1431.6599	1441.2557	1441.9781	1447.3444

```
1453.5602    1456.2239    1461.2175    1779.7090    2941.9223    2953.2932
2958.2575    2983.9807    2988.2454    3012.4611    3034.9156    3042.0900
3052.4344    3067.0132    3100.6856
```

```
==========================
         Structure    3
==========================
```

```
1440.0916i     44.3377      55.2696     109.0536     136.0711     165.3484
 181.9039     213.3897     256.9138     287.8788     323.6855     341.3863
 425.8751     483.3224     643.9658     685.1941     738.9897     828.4977
 839.2501     898.2388     942.8925     972.8534    1038.6126    1057.2392
1065.1703    1116.2599    1140.6437    1146.9990    1173.3810    1207.8829
1233.0807    1240.9745    1265.3158    1315.5094    1330.9980    1367.3209
1376.8911    1388.7257    1431.2527    1440.5225    1442.0905    1447.9461
1455.5025    1456.1356    1460.3817    1776.7579    2956.1869    2967.0960
2968.7075    2984.0712    3008.1068    3026.1027    3034.4325    3039.7266
3063.7864    3067.0824    3100.9959
```

```
==========================
         Structure    4
==========================
```

```
1433.3626i     46.6092      78.2988     108.6432     136.0846     161.8532
 200.5770     223.9765     282.7411     287.3571     304.9315     342.2402
 425.6560     479.0853     644.0493     687.2490     753.5507     817.8086
 854.0619     903.7830     926.6437     975.1250    1040.8006    1060.4932
1070.0970    1108.5217    1146.9269    1158.3696    1172.5849    1205.4904
1235.8792    1244.8853    1257.8523    1313.7490    1334.6356    1359.6308
1381.4908    1387.7191    1433.4374    1439.1708    1441.8926    1444.4198
1453.1744    1456.1050    1460.2510    1778.9418    2953.0477    2959.2847
2970.7029    2984.1471    2996.0776    3024.0012    3033.9461    3046.8584
3048.8574    3067.2757    3100.9041
```

```
==========================
         Structure    5
==========================
```

```
1445.5661i     31.5706      60.3453      96.2693     128.8428     142.3301
 173.0989     233.1042     267.1956     295.0666     308.4332     332.8467
 407.4080     458.1933     669.9299     699.9282     739.9817     801.4270
 866.2916     900.0825     931.9830     975.8667    1042.3469    1065.6412
1077.0781    1107.9003    1146.9626    1157.4792    1172.0420    1204.5883
1225.1938    1231.4905    1262.1026    1314.2948    1332.6062    1357.4100
1377.9791    1392.8206    1431.7987    1441.4810    1441.8531    1444.7075
1454.8567    1456.2080    1461.7567    1779.5679    2938.8379    2957.1362
2961.4275    2983.9699    3002.8258    3022.3864    3033.7128    3040.5166
3065.3151    3067.0115    3100.6913
```

```
==========================
        Structure    6
==========================


  1440.8715i      51.2818       67.3544       89.2526      137.1761      165.3476
   187.1429      209.5373      240.8454      279.5029      306.9762      332.2083
   414.1925      527.2588      613.0986      687.8514      730.7402      837.6461
   847.6341      873.9407      923.1531      998.6152     1036.7634     1060.9235
  1086.4947     1115.0645     1147.4208     1157.4722     1178.6096     1221.5300
  1228.5710     1256.1325     1285.6219     1292.5601     1334.1284     1356.4924
  1373.3375     1376.9084     1431.7554     1441.4974     1441.9053     1446.1608
  1453.0804     1456.0742     1459.3368     1779.3666     2956.5211     2957.4368
  2968.8211     2984.2606     2995.3674     3022.1403     3035.7992     3041.6657
  3064.7212     3067.6732     3100.1273


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        Structure    7
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  1452.1785i      47.8142       66.0550      107.2654      133.4206      156.6320
   195.6499      222.9376      238.4400      285.9814      296.4239      334.5824
   373.0489      549.1253      645.9020      673.7217      722.5540      830.2541
   836.4299      895.5852      926.8362     1005.6568     1041.2979     1057.6572
  1067.5873     1108.9755     1146.6988     1150.9099     1175.1593     1214.3976
  1223.0577     1237.2757     1272.4861     1287.5700     1358.0824     1366.7507
  1375.4022     1390.8357     1423.3353     1440.3413     1442.1877     1449.4798
  1453.9758     1456.3363     1460.1738     1777.5945     2943.7899     2954.8594
  2964.6462     2983.9798     2996.7531     3020.0447     3040.2767     3042.2620
  3055.1879     3066.9132     3100.8551


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        Structure    8
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  1444.0808i      49.8629       71.4495       98.3025      108.0753      139.0538
   171.0752      234.7043      236.9544      300.5907      320.0083      324.5650
   345.3163      498.6677      664.8049      705.9677      712.7478      802.9218
   866.8052      890.8565      913.9225     1020.6368     1045.7034     1069.3730
  1085.7881     1112.9653     1147.3120     1164.4369     1178.7810     1219.8116
  1229.9322     1232.1822     1280.5691     1291.4676     1327.7171     1362.0025
  1373.2303     1378.8415     1432.6219     1436.4325     1441.6298     1447.2067
  1453.7871     1455.8586     1460.8702     1779.4867     2939.7553     2954.7130
  2957.8837     2984.5569     2989.3688     3012.3926     3034.3450     3042.3323
  3062.4245     3068.1160     3100.4108


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        Structure    9
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   1449.8561i       48.5461        65.7849       100.7945       133.0282       143.6245
    177.5657       233.1238       262.0603       299.1383       327.7208       355.3438
    409.6803       442.1108       678.8386       696.8260       744.5048       799.8219
    867.4636       911.1349       923.9237       975.1640      1043.3061      1064.6364
   1078.2533      1108.6371      1147.0157      1153.8127      1172.4429      1204.3225
   1217.5722      1222.1395      1260.3280      1313.5593      1336.2759      1374.7825
   1379.2262      1390.5070      1428.2298      1439.8888      1441.9463      1444.9899
   1454.1290      1456.2918      1461.1842      1780.7689      2953.8720      2958.7690
   2960.4022      2984.0132      2996.1357      3005.3764      3035.9541      3041.8541
   3044.5199      3067.0755      3100.6959

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                            Structure   10
                        =========================

   1440.3116i       47.7008        51.5247       104.7325       138.0174       166.9227
    178.6042       215.0658       260.0031       287.0929       322.0223       343.9001
    449.6479       503.3117       610.7762       696.9779       739.9620       833.1068
    839.1519       876.3168       930.5082       974.3370      1032.4668      1062.6984
   1085.0347      1115.0740      1139.7483      1147.3325      1178.1287      1214.9348
   1232.8986      1254.4271      1280.9419      1315.0852      1329.2966      1355.4154
   1372.1844      1380.4662      1431.4538      1440.2906      1441.5609      1446.8080
   1455.6772      1456.3189      1461.0232      1778.5194      2957.9693      2962.3244
   2967.9133      2984.2224      3002.8760      3026.2394      3035.2330      3042.4101
   3067.5446      3074.5614      3100.2112

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                            Structure   11
                        =========================

   1434.3140i       55.7619        69.9699       100.1903       136.4121       169.7076
    199.7616       222.8144       288.6864       293.2648       300.1411       337.7198
    452.3658       493.6186       614.1810       693.8614       756.6141       818.3427
    857.2807       873.8577       917.5639       976.2187      1035.0385      1064.0164
   1086.1383      1110.8334      1146.7414      1159.2114      1178.2609      1214.0174
   1233.9411      1257.4057      1279.5486      1313.1197      1333.1251      1356.9947
   1364.1254      1381.4893      1432.2780      1440.5976      1441.3844      1444.2830
   1455.3939      1455.8164      1464.6274      1776.6139      2955.6425      2958.9741
   2971.3984      2983.7537      2996.8485      3025.1700      3037.5120      3041.3078
   3059.7165      3067.0578      3099.6887

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                            Structure   12
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   1444.0622i       30.1325        66.3297       103.5323       124.6838       140.3941
```

173.6385	219.9120	264.6343	299.3446	312.0037	329.4840
415.6812	470.5212	654.0093	705.9562	739.0012	799.7901
861.6662	878.4252	921.8561	984.5737	1042.7872	1075.9340
1085.8246	1107.9888	1147.2880	1155.7169	1177.7904	1222.5495
1229.5655	1237.3331	1277.6996	1306.7194	1331.7140	1361.7521
1368.8496	1379.8818	1432.0829	1436.1090	1441.3443	1444.1021
1455.0762	1455.8597	1461.6158	1778.7960	2937.5971	2959.3307
2960.6588	2984.4904	3002.3133	3021.6011	3036.0229	3042.3619
3068.0888	3076.9821	3100.2587			

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Structure   13
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1452.0874i	45.3019	73.8298	103.3051	134.0592	143.6535
182.4258	227.2254	264.6659	298.4057	324.6688	357.9298
419.6604	467.4363	663.5411	706.5737	744.2776	800.8643
860.6282	877.4607	924.9058	980.6299	1057.2835	1068.5576
1084.9267	1111.5697	1147.4486	1154.7603	1177.9393	1216.8203
1221.2103	1237.7156	1273.1355	1302.6615	1335.0415	1365.7908
1371.9299	1380.8668	1429.4739	1436.1233	1441.6703	1444.3876
1454.1247	1456.0277	1461.4596	1780.9944	2952.5450	2958.2369
2959.2203	2984.5675	2995.0179	3005.3556	3036.3868	3043.0233
3057.0619	3068.1460	3100.4246			

==========================
Structure   14
==========================

1457.7024i	46.8795	97.5771	126.7941	141.4796	173.1983
208.5036	242.4261	290.9874	306.1452	326.5579	357.9501
399.8410	521.9605	648.7930	665.2426	757.9823	804.6670
855.8382	898.3692	934.7173	973.7235	1042.7392	1070.1124
1077.1220	1096.3543	1143.3044	1147.7518	1174.5263	1209.7557
1228.5652	1236.7646	1263.8404	1324.0961	1331.5906	1362.1602
1380.7008	1384.0820	1428.7678	1439.1550	1442.3577	1442.9863
1451.8467	1456.3803	1458.3838	1778.5815	2954.8109	2963.1598
2964.1404	2983.8545	3000.1057	3020.2571	3038.7659	3051.0554
3057.4684	3066.8782	3100.5876			

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Structure   15
==========================

1456.8488i	31.7725	64.1834	132.4904	148.8512	167.1324
203.5088	252.8506	281.9741	298.3952	320.6188	354.0440
389.1939	524.9576	665.6508	693.7837	736.6346	811.8904
829.6647	900.5444	924.9601	970.8368	1037.0031	1058.3400

1073.5752	1116.6426	1142.3265	1147.2712	1173.3752	1213.0605
1233.2452	1252.5675	1269.3968	1331.0653	1352.5466	1364.8625
1378.0001	1389.4222	1425.1387	1440.5653	1442.0848	1444.5875
1452.2736	1456.3871	1462.5413	1777.6167	2943.4009	2954.5104
2972.4210	2983.6981	2984.6786	3024.4863	3040.5177	3049.5931
3050.6366	3066.4312	3100.4533			

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       Structure   16
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1461.1254i	44.9730	63.2286	97.5381	134.7094	160.3340
192.2052	221.7281	241.2530	298.0533	303.7441	340.0333
375.3430	578.4059	611.1435	682.1398	719.6747	826.4320
844.4001	869.0645	920.2687	1006.6848	1043.7727	1066.4327
1080.7422	1105.5169	1146.9759	1151.4555	1178.7302	1219.1426
1228.9873	1266.6019	1285.5259	1287.8786	1332.0131	1357.1355
1373.8989	1375.8585	1426.2890	1437.6487	1441.2112	1448.5348
1453.5745	1455.7937	1460.2832	1777.6604	2944.9710	2955.2690
2966.9868	2984.8560	2995.5207	3017.4018	3037.5162	3040.6101
3067.1353	3068.8673	3100.0013			

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       Structure   17
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```

1451.6593i	25.5059	88.9689	131.6783	148.0312	180.5841
203.3782	249.3724	281.1135	291.2183	320.5084	354.0422
401.6689	552.8750	627.6513	729.8463	738.6218	803.7310
834.6386	870.7435	917.8766	974.1567	1034.3998	1059.8065
1093.7398	1110.9416	1141.0515	1146.4940	1178.8827	1222.7963
1250.1761	1265.5074	1290.9164	1327.0718	1334.4870	1359.3795
1377.5016	1387.7088	1426.8576	1436.4568	1441.3342	1448.2157
1453.5175	1456.4552	1464.8035	1773.1977	2940.2123	2957.6735
2971.2964	2982.2374	2984.8700	3024.6874	3040.2190	3050.5782
3064.8774	3068.8438	3099.9831			

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==========================
       Structure   18
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```

1462.8952i	35.5645	71.1332	128.6269	144.2916	184.8793
204.0420	236.8757	287.9662	316.0273	326.1453	360.9731
418.7914	533.8563	620.3196	673.4461	758.9973	801.7032
864.0934	869.9000	924.7765	984.9080	1044.2472	1079.6713
1087.4919	1092.0257	1147.1109	1149.1922	1178.8901	1218.3339
1245.5329	1259.8204	1280.2174	1324.3220	1325.5362	1337.4575
1358.5650	1382.2777	1431.5605	1437.2255	1440.9798	1443.3108

```
1451.2462    1455.9197    1456.0599    1776.1720    2956.6525    2962.9208
2968.3112    2984.6585    3000.8147    3019.8108    3041.4299    3043.9960
3068.3346    3068.5131    3099.7822
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          Structure   19
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```
1465.3567i     37.4595      51.6495     100.3867     132.9000     154.2339
 181.4588     200.0162     271.6933     300.6366     335.6343     356.4656
 413.7617     540.6008     616.5902     686.8773     748.7415     822.3751
 835.3197     877.9612     916.6806     980.5902    1039.5348    1064.8713
1083.3813    1103.5970    1138.9987    1147.1357    1177.9325    1208.2327
1232.6388    1255.5731    1278.8466    1319.1941    1332.3688    1346.3903
1376.6289    1386.2395    1427.2445    1437.2061    1441.2764    1447.4620
1454.0335    1455.7894    1459.4337    1779.1570    2955.9595    2959.1391
2973.5818    2984.7842    3004.1061    3016.5191    3037.4516    3044.2710
3068.5122    3068.6698    3100.1955
```

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          Structure   20
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```
1450.5238i     61.9028      76.9765     103.9796     135.3880     204.4356
 209.7639     231.7508     241.0793     271.5769     297.1333     355.9915
 418.3009     551.7184     579.7331     653.3912     715.5172     786.2381
 847.6469     881.2039     924.8495    1022.9056    1051.1655    1069.5261
1081.7093    1114.9352    1140.1419    1149.6898    1169.8001    1213.7885
1226.3292    1247.1316    1268.6476    1289.9921    1339.8049    1370.6654
1373.7171    1383.1815    1431.8549    1447.1808    1447.7857    1453.3274
1457.7436    1459.1016    1463.0044    1793.7613    2953.5611    2957.2810
2963.3407    2967.1536    3008.7626    3025.4523    3037.2950    3041.9655
3043.2040    3043.8954    3087.0205
```

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==========================
          Structure   21
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```

```
1453.2242i     62.5424      78.3453     108.2505     127.6096     138.3615
 207.6614     236.4062     245.7075     289.7436     300.5444     337.9156
 394.4313     535.6180     588.5119     653.9809     709.7800     804.8078
 848.0856     892.6540     915.0632    1030.8576    1054.7635    1074.4786
1083.1708    1115.0832    1139.7552    1148.1341    1173.1642    1206.3179
1222.4683    1230.4765    1264.1401    1278.3997    1344.4537    1364.4639
1377.4866    1392.7621    1428.6937    1446.5417    1447.7394    1453.6812
1457.4475    1461.0232    1462.8222    1796.7718    2947.1828    2953.7583
2959.4212    2963.0814    2986.3910    3015.4431    3036.0645    3038.2364
3043.0947    3043.3187    3086.7312
```

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                             Structure   22
                        =========================

    1451.4357i        53.0108        62.3595       120.0451       139.5374       202.0032
     210.6187        224.5687       258.0898       292.2985       323.8256       343.8662
     447.5799        531.1011       579.1034       655.1829       725.8154       790.9393
     832.5775        878.9084       936.3253       982.2929      1058.7116      1064.2684
    1081.6191       1116.9393      1139.9095      1149.4343      1151.9518      1209.5880
    1230.4893       1242.3777      1265.9582      1315.2958      1329.9242      1364.8136
    1375.5111       1386.4087      1430.3924      1447.2673      1448.2607      1455.4134
    1457.6732       1459.6474      1462.9517      1793.3468      2954.5988      2962.7760
    2966.5299       2972.9782      3013.4701      3029.3858      3036.4534      3039.9093
    3043.1006       3052.7191      3086.7878


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                             Structure   23
                        =========================

    1456.6991i        66.0655        68.2506       114.2107       132.9340       202.1337
     221.9844        226.1471       239.5286       269.0395       303.1317       369.3163
     425.0915        555.7821       601.7682       646.8418       707.9618       785.1278
     842.9339        873.0677       923.1959      1022.8615      1056.0645      1060.6395
    1082.7819       1112.7927      1139.7131      1150.0859      1162.4182      1213.6668
    1222.8636       1237.5920      1273.7905      1288.0739      1355.5822      1367.0938
    1375.4522       1390.6036      1420.7272      1447.3972      1449.0397      1454.2396
    1457.5883       1459.4940      1463.0338      1794.2983      2948.6555      2955.5186
    2963.4446       2964.6489      2999.2171      3021.4260      3041.5902      3042.1095
    3044.2414       3046.7034      3087.4467


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                             Structure   24
                        =========================

    1454.1393i        34.9631        87.9006       115.7462       131.9664       144.7889
     208.6769        241.7309       267.8724       291.3549       305.8070       346.9412
     431.6443        510.6527       590.6994       652.8166       730.4198       799.4748
     850.3366        874.3381       924.6839       987.7427      1057.8354      1073.4787
    1090.6879       1110.4575      1139.7789      1147.7837      1163.1901      1208.9706
    1221.9582       1228.6916      1262.0355      1310.4279      1333.1447      1362.9151
    1378.1903       1391.1797      1429.2278      1444.1624      1447.2745      1455.0194
    1457.6183       1461.7883      1462.9132      1796.4936      2947.7454      2957.2541
    2961.3518       2962.7349      3003.0883      3025.5805      3033.1321      3040.3530
    3043.1410       3053.1549      3086.5160


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                             Structure   25
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 1445.1513i      54.5986        91.3536        115.8062       137.2191       209.1111
  214.8277      231.3630       281.3643        291.5418       312.9226       343.3624
  451.0234      528.2859       573.1596        649.5975       748.5105       774.8647
  846.6490      882.9727       920.9252        985.4368      1062.5036      1071.4379
 1082.7570     1110.0025      1139.9052       1147.6480      1167.2773      1206.5807
 1235.0939     1244.6043      1257.9151       1311.6249      1335.1110      1353.2755
 1382.0625     1385.1190      1431.5121       1441.7905      1447.4495      1452.5670
 1457.4212     1458.0076      1463.2551       1795.1830      2949.2346      2961.8392
 2962.7110     2971.5947      2995.4688       3027.9194      3034.8314      3039.6837
 3043.1185     3051.9730      3086.4460

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                             Structure  26
                        ==========================

 1457.1374i      52.8327        97.5156        111.9854       130.4453       174.3914
  207.5918      244.0570       257.8284        306.4785       326.1756       359.9240
  430.6247      508.0654       591.4135        655.0409       734.4405       801.9952
  857.2785      874.8995       922.4228        985.7042      1060.8637      1078.8983
 1086.4967     1108.7979      1139.7895       1146.4737      1161.2969      1208.3589
 1214.7265     1225.5449      1258.2135       1309.9045      1335.9331      1374.1436
 1378.9543     1389.0652      1426.3665       1444.0722      1447.0638      1454.0619
 1457.7615     1460.6045      1462.6730       1798.0451      2953.2337      2958.4131
 2963.2024     2966.5691      2998.8344       3009.1187      3032.0965      3035.6634
 3041.0338     3043.7454      3086.8445

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                             Structure  27
                        ==========================

 1462.2514i      67.1189        98.5719        132.5036       165.6207       203.6763
  219.6471      252.5893       295.6027        305.5236       323.7306       392.3334
  458.9641      547.7511       572.0377        641.6603       751.4961       775.0677
  837.0341      882.7916       928.6994        985.6575      1068.3780      1076.0087
 1080.7074     1104.6821      1139.4302       1148.2783      1158.0028      1215.4962
 1223.5973     1236.9847      1264.4252       1324.6653      1332.3676      1361.8454
 1377.0491     1385.1575      1428.1428       1441.7405      1447.2257      1452.1487
 1457.6545     1457.7627      1463.0752       1795.6951      2952.9456      2964.1396
 2965.0611     2969.1676      3000.1567       3022.9678      3038.5999      3045.8559
 3047.3601     3054.6665      3086.8920
```

S.3.4 $(\mathbf{TS}_\beta)^\ddagger$

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Structure   1

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1269.2464i	31.7575	69.1952	82.3303	136.0357	164.7554
172.2349	223.8808	238.3545	276.7639	302.6056	343.6161
358.6349	510.3167	570.3361	671.7425	735.7837	826.4567
837.7258	901.7789	921.9218	1004.0827	1029.0712	1056.8795
1089.6168	1098.5697	1144.6622	1170.2516	1173.4621	1179.8442
1196.3157	1223.0276	1247.9412	1278.4696	1341.1965	1369.5091
1382.5351	1404.7632	1430.1820	1433.7299	1439.7132	1450.5575
1452.9318	1454.6717	1577.8691	1792.0666	2932.3449	2954.5087
2965.9528	2971.4913	2979.1188	3009.7463	3029.3232	3032.1342
3038.7335	3062.7044	3095.4280			

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Structure   2
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1299.8156i	33.3845	62.8891	96.2159	112.0544	135.9666
173.5871	224.2910	245.7023	285.8526	309.0656	325.3670
350.7900	476.4314	573.3942	690.4728	737.6066	813.4152
880.6014	910.1294	915.6372	1011.5085	1038.5920	1063.9839
1079.9711	1108.2651	1145.0473	1156.1585	1169.2675	1180.2994
1197.5241	1211.0944	1245.8065	1263.7948	1340.2012	1373.2261
1392.1815	1401.2773	1431.0397	1436.9248	1439.4687	1450.0593
1453.0761	1455.2897	1543.2157	1799.5797	2916.2763	2932.2449
2956.0804	2965.8875	2978.8767	3001.6593	3033.1831	3039.4789
3040.5669	3062.5375	3095.0734			

==========================
Structure   3
==========================

1267.8997i	30.6630	43.0796	116.6907	137.1352	159.3068
169.7191	226.2503	268.0335	283.9919	288.1064	351.9456
436.6322	485.2825	573.7832	672.6342	737.8179	816.4516
838.8909	901.8431	928.9933	965.5394	1028.4965	1057.1578
1072.5881	1109.1922	1144.5544	1159.4333	1170.5680	1184.0808
1197.5096	1218.6184	1247.0961	1322.0951	1329.7393	1364.2665
1377.8677	1408.3236	1431.2091	1433.4753	1439.5170	1451.4483
1452.8913	1458.8327	1573.1272	1791.5354	2944.2066	2953.3299
2971.9166	2979.0034	2987.9364	3017.6604	3029.3554	3037.0205
3038.6726	3062.5057	3095.3572			

==========================
Structure   4
==========================

```
1299.1167i     36.2211     51.9029     98.4331    134.8066    142.1034
 173.3032    230.4952    238.1979    277.3355    312.8183    322.7502
 418.0112    477.6328    571.4334    692.2829    744.6917    815.2809
 867.9906    904.9561    921.8955    968.5627   1036.4280   1061.3830
1075.6003   1113.5716   1144.9233   1147.8497   1170.5105   1187.6055
1201.5989   1209.7948   1242.3255   1300.0981   1324.7893   1372.9595
1389.6865   1401.7150   1429.1186   1436.5275   1439.4011   1451.7255
1453.1071   1457.4689   1543.1416   1799.2894   2916.8079   2927.5920
2955.2827   2978.8486   2986.7336   3007.3414   3032.2293   3038.5200
3049.3405   3062.5026   3095.0749
```

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                    ===========================
                         Structure     5
                    ===========================
```

```
1298.2190i     33.6985     45.9640     98.4803    128.4350    137.2558
 172.9186    216.9853    232.1099    279.0724    312.8499    340.9141
 419.2491    431.9146    574.1869    694.0908    747.7578    809.9278
 873.1522    904.7599    932.2293    966.4672   1034.0145   1049.9080
1089.0919   1111.8608   1145.0004   1152.9095   1170.1690   1183.0626
1197.9869   1213.1961   1250.7780   1296.4696   1325.2285   1365.7394
1389.9453   1401.8927   1435.9531   1438.3107   1439.4251   1450.6068
1453.0733   1455.5448   1547.7973   1799.1201   2936.9292   2951.2985
2953.6881   2978.8749   2994.5751   3002.3773   3032.4136   3034.1060
3041.4418   3062.5374   3095.0739
```

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                    ===========================
                         Structure     6
                    ===========================
```

```
1283.4046i     22.4985     59.8848     74.1592    136.8240    162.3736
 176.3670    223.2033    243.0475    281.0220    303.9738    350.9374
 373.3081    501.2957    593.5286    674.5822    736.0547    826.9428
 841.1481    871.6633    924.4645   1003.8388   1039.0719   1060.0941
1091.0908   1097.6936   1144.9799   1171.4809   1174.0096   1182.7134
1196.8105   1247.6553   1256.5162   1295.8036   1298.6036   1367.9084
1377.9540   1412.0999   1427.2590   1431.9154   1439.0737   1450.4074
1452.7719   1454.7895   1563.2694   1796.5947   2918.0919   2955.2101
2968.4670   2971.2454   2979.0462   3026.8890   3032.1022   3039.6985
3040.9928   3062.7829   3094.9152
```

```
                    ===========================
                         Structure     7
                    ===========================
```

```
1296.3563i     24.1917     79.6776    115.4590    138.9092    142.5808
 200.2431    232.4130    254.4030    285.5185    300.4639    375.8555
 416.1500    482.1773    619.4828    736.3417    750.8829    815.7873
```

835.5224	894.3201	932.3138	963.5337	1031.6777	1059.1462
1086.2208	1097.1629	1144.6280	1150.9036	1172.3894	1180.6113
1201.6188	1245.6869	1250.8626	1314.1061	1327.8354	1342.4377
1374.4824	1421.9129	1427.7361	1436.8637	1439.1638	1448.4376
1452.4179	1466.7981	1523.3441	1787.2286	2933.2956	2955.5362
2978.9821	2984.3158	2996.1479	3022.0321	3032.8576	3047.0552
3058.2628	3062.5409	3095.5271			

==========================

Structure   8

==========================

1271.2510i	26.6269	74.4201	92.4402	136.4512	160.7970
181.7561	228.7784	242.2189	284.6866	302.8574	356.9956
404.2235	477.9181	569.6633	678.2676	753.2814	816.3274
856.1003	907.9190	914.0425	968.3684	1031.6577	1048.5976
1087.2175	1107.9585	1144.7737	1169.8154	1173.7272	1181.9787
1192.7811	1220.2696	1255.1828	1297.9977	1327.5906	1366.1091
1380.4536	1405.0169	1433.8160	1436.5751	1439.7089	1446.3504
1452.7765	1453.2879	1579.1269	1793.3353	2947.7105	2952.8423
2953.6452	2979.1976	2995.1740	3014.5678	3028.9269	3038.3696
3044.4080	3063.0075	3095.5201			

==========================

Structure   9

==========================

1289.7675i	22.4172	58.4703	69.9429	132.4529	147.4598
194.2082	225.7237	241.6648	280.2374	302.5576	346.2382
406.8935	432.5481	621.4261	734.2342	750.1369	823.8630
851.2730	881.5086	928.5519	994.5280	1036.7355	1058.4335
1086.3612	1092.8341	1144.5250	1164.3224	1171.1486	1179.0082
1195.1403	1245.5442	1256.6537	1278.0603	1322.2651	1365.3264
1374.7304	1421.5592	1427.7123	1435.6587	1438.9951	1450.4565
1452.5326	1455.1106	1541.4464	1791.6717	2927.0148	2955.4945
2973.5742	2979.0140	2987.9851	3020.6141	3032.5383	3040.1905
3051.5650	3062.4643	3095.5934			

==========================

Structure   10

==========================

1301.2653i	31.2495	60.5359	98.6693	103.2595	137.7623
180.6610	222.9722	239.0879	285.7425	315.8708	326.6269
356.0396	469.3871	599.5222	681.1229	738.3064	804.9224
864.4107	892.1287	915.5006	1020.2187	1049.9917	1064.9954
1079.6104	1106.8064	1145.1648	1160.4283	1174.6591	1185.4814
1202.9917	1222.8731	1247.0458	1295.3810	1320.7777	1370.6740

```
1377.2685    1404.2435    1431.2279    1433.0767    1438.9190    1450.2840
1452.2961    1454.9720    1541.1469    1798.3099    2916.7020    2930.7913
2955.6192    2969.2842    2979.6989    3023.1567    3032.2430    3039.6731
3040.8213    3064.0029    3095.2538
```

===========================
Structure   11
===========================

```
1294.7914i     32.0227      73.9540     112.2053     137.2138     147.3462
 204.8488     233.5144     249.1265     285.6405     297.1366     369.4775
 419.9201     480.4332     618.2895     734.5880     750.8727     815.9752
 850.5414     868.9713     940.4553     959.8011    1031.9909    1057.4942
1084.4538    1101.7767    1144.3979    1152.2508    1170.1331    1179.5415
1199.1022    1243.7903    1257.7787    1307.1663    1327.0220    1343.3351
1373.9924    1422.1158    1429.0591    1434.7283    1438.6929    1449.4563
1452.9606    1464.8095    1530.4634    1793.6604    2929.0536    2956.8375
2978.9213    2984.1967    2995.3696    3026.9792    3033.7119    3044.4968
3058.4032    3062.4873    3095.0527
```

===========================
Structure   12
===========================

```
1314.8236i     29.7533      66.4791     113.9821     138.8545     165.8076
 180.3332     219.9988     234.3899     280.5305     291.3692     347.5874
 365.2058     524.9438     566.0851     674.7677     734.9903     819.5398
 835.8091     902.4151     918.7460     999.3383    1034.5676    1044.3580
1063.5052    1114.5521    1144.7517    1150.1609    1171.3219    1174.2460
1203.3767    1226.4760    1247.9162    1270.2434    1362.5029    1367.0279
1376.1934    1396.9404    1433.8364    1434.6689    1439.4668    1450.3371
1453.3543    1454.8457    1592.3700    1801.0461    2907.8458    2942.5492
2952.7182    2978.4959    2999.0076    3006.7159    3017.0583    3033.2282
3039.2445    3061.8264    3094.5750
```

===========================
Structure   13
===========================

```
1288.7132i     41.3203      50.1967      79.1761     136.2574     153.9612
 188.9155     236.4989     247.4226     281.5500     301.6411     366.3484
 402.7168     484.0496     591.4220     683.9085     754.9081     814.0250
 849.1264     883.6725     917.0097     974.0112    1037.0479    1050.7224
1094.8488    1104.8226    1144.3440    1173.9908    1175.4981    1187.1388
1197.7866    1249.1280    1272.4620    1298.4818    1304.7438    1363.5195
1369.9139    1410.6054    1431.3895    1437.3169    1438.9339    1446.7898
1452.1094    1461.4517    1546.8815    1793.6614    2951.7920    2953.4726
2961.3433    2978.0426    2994.5464    3028.0757    3033.3625    3036.6999
```

```
3042.7434      3061.5800      3094.3860


                    ==========================
                          Structure   14
                    ==========================


   1300.2471i       30.6394        50.8692        91.8669       126.6292       139.1122
    188.3470       208.2486       233.6196       275.0217       310.8756       342.8552
    411.3803       456.7955       594.2075       687.5507       748.8120       802.9617
    862.2661       881.1809       930.1723       969.7773      1048.7818      1050.5530
   1093.8797      1110.2593      1145.1293      1158.2390      1174.7200      1188.5226
   1203.0383      1225.8236      1272.8032      1304.1109      1308.5822      1365.1770
   1369.6881      1406.2834      1432.9083      1437.7101      1438.9250      1450.6295
   1452.3305      1456.1736      1547.6862      1798.2710      2935.2772      2952.5275
   2953.3726      2979.5908      2995.6074      3022.8772      3032.7834      3034.5528
   3041.1787      3063.8869      3095.1123


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                          Structure   15
                    ==========================


   1309.7275i       26.3788        48.2326       122.6608       142.5799       166.4344
    176.1035       228.8889       237.2544       277.1527       292.3750       356.0670
    426.8868       485.5816       565.3177       675.2726       745.0278       814.5463
    838.0936       899.4344       926.8306       959.8304      1033.1230      1039.1751
   1066.3600      1113.6433      1144.3480      1147.5023      1171.0365      1172.5789
   1198.5651      1222.6394      1251.6766      1297.5101      1356.8733      1362.0245
   1367.9562      1399.3885      1434.6459      1439.4979      1443.5671      1451.7291
   1453.3022      1456.8797      1603.4804      1800.3721      2948.9235      2952.2170
   2969.0926      2978.4596      2996.6371      3008.5998      3018.3568      3031.4487
   3037.9576      3061.7411      3094.5774


                    ==========================
                          Structure   16
                    ==========================


   1301.1569i       24.5661        51.2745       102.2132       126.1845       138.9887
    185.9822       223.5596       233.5457       277.9356       305.9446       324.6508
    436.0726       468.4390       590.2364       689.3065       742.6969       805.3144
    862.1228       879.2656       919.6425       975.8299      1046.1354      1060.3982
   1083.5970      1111.8404      1145.1236      1150.0480      1174.6468      1192.4982
   1205.5249      1231.6271      1253.5504      1302.4786      1328.2552      1365.6966
   1375.9092      1405.7263      1428.7224      1433.1116      1438.7662      1451.4657
   1452.4114      1458.3182      1543.4890      1797.8501      2917.2453      2923.8076
   2957.3502      2979.6280      2985.3550      3031.9222      3037.5904      3040.3435
   3050.9257      3063.9434      3095.1116


                    ==========================
```

```
                        Structure   17
                   =========================

  1315.6860i       30.3401       68.9272       88.0445      137.2920      166.8936
   182.2963       221.2575      242.9457      285.3930      305.2944      365.2634
   371.7219       511.2171      592.4719      701.0698      736.0039      821.0887
   839.5312       873.2954      923.4222      992.8209     1019.7263     1059.9525
  1078.1914      1110.2874     1144.9696     1152.5640     1173.8125     1181.2800
  1195.7081      1243.5419     1258.2193     1283.4782     1331.7270     1365.9807
  1375.4885      1407.2927     1427.9784     1434.1983     1439.5062     1450.1974
  1452.5142      1454.8778     1595.7599     1795.5390     2918.2540     2955.0129
  2960.4372      2977.6258     2978.4672     3009.1186     3013.6677     3031.7363
  3040.5450      3060.6966     3095.4184


                   =========================
                        Structure   18
                   =========================

  1312.5822i       23.1024       70.2419      108.5046      137.5625      142.2227
   185.8087       236.8747      253.3316      275.9491      291.0424      385.8688
   428.4128       462.0032      605.6865      730.8006      745.9165      818.2815
   837.1917       883.1380      930.7180      952.4988     1021.0740     1064.2250
  1072.6921      1107.8656     1143.7925     1144.6886     1173.0268     1178.7223
  1190.3227      1233.8755     1273.3299     1297.7811     1319.3033     1357.6716
  1369.1472      1414.4357     1435.1458     1439.1178     1441.8623     1451.2271
  1452.4394      1460.3580     1594.8857     1793.6066     2949.8278     2953.1691
  2970.3962      2977.9084     2995.0006     3018.8014     3021.7336     3031.5445
  3041.3849      3060.5493     3095.8423


                   =========================
                        Structure   19
                   =========================

  1329.2605i       31.1855       74.2314      118.2016      137.9124      141.8363
   201.1141       231.8564      245.3251      277.5505      294.3454      407.1878
   422.0607       433.0483      609.1752      741.2743      753.9704      816.8336
   844.9581       873.0311      932.0928      961.2161     1031.0994     1044.4045
  1080.9602      1106.2704     1137.9359     1144.7115     1171.6787     1182.0663
  1192.3502      1234.3413     1267.7624     1297.0008     1321.6023     1357.4794
  1364.0486      1418.0970     1435.3017     1438.7056     1440.5564     1449.8106
  1453.0351      1460.9102     1586.4191     1802.2407     2953.2008     2955.0838
  2966.4390      2978.5063     2995.5583     3018.2345     3030.4015     3035.3699
  3042.2445      3061.7848     3094.8241


                   =========================
                        Structure   20
                   =========================
```

```
1317.3379i      47.3373       61.2660       93.4980      142.4496      167.6008
 200.2260      236.1310      259.9694      297.7776      316.1286      346.4173
 405.1989      539.7551      585.6948      698.6076      750.9170      802.0117
 844.0454      873.7691      919.2518      968.0761     1019.1556     1068.1705
1076.5153     1096.7588     1144.4468     1148.2133     1173.9628     1180.3480
1192.8956     1249.1148     1280.4874     1306.1744     1331.2534     1353.9851
1376.2805     1406.0724     1427.7670     1433.8336     1439.5607     1447.6626
1451.7190     1466.1531     1612.9423     1791.2464     2918.5982     2958.6402
2959.2071     2975.2160     2983.7544     3008.8165     3021.6196     3037.4430
3042.4520     3057.7162     3094.6781
```

===========================
          Structure   21
===========================

```
1331.2754i      20.5055       80.6408      104.3802      139.5454      171.3678
 200.7745      228.4190      262.4651      308.9986      312.7979      348.5027
 394.7110      533.6037      572.2562      688.9809      744.8792      807.4834
 841.2190      904.9297      915.9020      963.6300     1034.8987     1045.0827
1070.6944     1095.1512     1143.0859     1145.2727     1168.5192     1173.2638
1190.3671     1230.8267     1251.4412     1327.4640     1334.3718     1354.8222
1377.8402     1402.2770     1428.0452     1433.1639     1439.1023     1448.5248
1452.9114     1461.2035     1631.1880     1803.7347     2913.2042     2949.1288
2954.0115     2978.2601     2980.8213     2997.8455     3026.5578     3027.7634
3047.9728     3061.6242     3094.3070
```

===========================
          Structure   22
===========================

```
1349.8119i      39.2838       56.2874      101.6637      136.4674      146.0483
 222.3260      249.8402      254.4582      288.1092      325.0303      354.5032
 406.9828      486.6925      615.8084      726.6544      761.3328      796.7827
 863.9769      880.2471      930.7429      960.6720     1031.2389     1062.3115
1085.0994     1096.2048     1144.1548     1162.0299     1176.7248     1179.1429
1210.8071     1242.9848     1268.6724     1309.2625     1325.0006     1326.6116
1378.3512     1422.1709     1427.1452     1433.5315     1439.1844     1448.6976
1451.1551     1454.2360     1506.9724     1799.2894     2917.1879     2960.3828
2977.7889     2978.5134     2986.5905     3032.5559     3040.8901     3041.1477
3054.3175     3061.7574     3094.0009
```

===========================
          Structure   23
===========================

```
1271.1957i      39.0488       70.2620       94.4089      114.1142      181.9538
 191.5074      226.0450      245.3446      256.9936      302.1845      355.8774
 407.2977      523.5752      548.7571      593.3103      735.2443      797.5500
```

833.2856	870.9428	923.2253	1011.0963	1056.1233	1076.8906
1087.2065	1102.1721	1135.5388	1144.1984	1176.1111	1182.7843
1199.6658	1221.6961	1248.6082	1280.4285	1337.8598	1369.3927
1380.4778	1399.5215	1429.8002	1442.7965	1450.7096	1453.1974
1454.5139	1458.7907	1574.9560	1812.9536	2934.1313	2951.3959
2955.0385	2959.9684	2973.2966	2997.3103	3031.6211	3034.8149
3037.4990	3039.8762	3081.5474			

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==========================
        Structure   24
==========================
```

1305.8917i	50.6285	70.9993	105.0242	118.1032	123.5451
195.7822	225.0484	243.3813	276.6142	313.8268	336.8200
399.1991	519.9837	538.7661	587.0525	737.6326	815.8055
839.8795	896.0937	916.7953	1023.9198	1060.5802	1076.6980
1085.2648	1106.4208	1135.7906	1143.7225	1156.3391	1174.4793
1200.5161	1213.1652	1246.6397	1259.6164	1338.2434	1373.6485
1387.7118	1397.3950	1430.9317	1442.9813	1450.1063	1453.1604
1455.2305	1458.6010	1551.0150	1821.2855	2914.6681	2922.0962
2956.9670	2957.2909	2962.7094	2982.4924	3034.6035	3034.8549
3040.6632	3048.7904	3080.2141			

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==========================
        Structure   25
==========================
```

1271.8106i	38.2688	44.6548	111.1925	135.7118	178.6523
193.8188	224.4630	257.1706	281.6478	299.2461	366.0251
467.6103	517.0727	540.5578	587.9826	736.9030	799.7145
822.2056	872.6484	928.7897	972.1358	1052.9016	1068.1798
1084.7938	1111.8975	1135.5058	1143.5863	1162.7374	1187.4545
1203.0898	1218.2983	1248.3176	1320.6616	1330.6716	1361.5537
1376.5785	1402.5781	1431.6538	1442.6354	1450.4846	1453.2043
1458.1933	1459.9436	1566.1666	1812.1573	2949.3101	2952.4377
2956.5694	2961.1065	2990.8174	3005.4068	3026.8422	3036.9630
3037.8959	3041.4491	3081.1825			

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==========================
        Structure   26
==========================
```

1304.9295i	44.0635	73.8171	102.8718	118.8347	150.1292
197.6176	237.8014	245.7951	271.1636	314.2289	332.9115
477.5775	502.3862	531.5822	592.1895	739.8432	816.0959
846.7420	879.1930	920.7399	977.4633	1057.5830	1069.8036
1089.5223	1111.2985	1135.8128	1144.6725	1146.3546	1183.4199
1207.4053	1211.4650	1241.7692	1294.5015	1324.9932	1372.4376

```
1385.9559    1396.8523    1429.3581    1442.8935    1451.4065    1453.5113
1457.3621    1458.8638    1549.7404    1821.2268    2916.6525    2917.9569
2953.8921    2957.3053    2986.9978    2989.3356    3029.3992    3034.7525
3038.8226    3058.8822    3080.1442
```

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==========================
        Structure  27
==========================
```

```
1304.2073i     38.7507      69.2677     105.8368     120.1171     139.6663
 197.9261     222.9718     232.2668     276.3170     314.2229     359.7870
 427.4402     501.9587     532.9287     589.9713     745.9612     814.8408
 842.1895     881.7901     931.9624     974.7444    1048.3183    1076.7456
1093.3917    1108.6655    1135.9468    1142.7578    1154.0626    1177.2737
1202.6386    1215.2112    1249.2790    1295.1015    1322.7824    1365.9756
1386.3983    1397.0231    1437.5212    1442.9839    1450.8474    1453.4107
1455.1560    1458.9078    1555.8986    1821.0121    2927.0387    2949.7912
2953.4946    2957.2470    2982.9642    2994.5779    3030.9451    3034.6799
3035.5377    3050.0399    3080.1252
```

```
==========================
        Structure  28
==========================
```

```
1275.2593i     41.6587      87.2521     100.8548     124.5475     188.4710
 196.1024     222.5247     251.7802     287.6596     299.6228     379.6167
 435.8348     518.0973     532.2288     582.5997     753.3463     794.9733
 833.4248     885.8020     916.6521     977.1840    1049.6860    1078.6870
1090.9439    1109.2225    1135.7134    1144.5667    1175.9816    1186.4579
1199.2880    1217.0432    1258.1916    1296.6129    1326.3225    1368.7294
1377.6006    1398.8839    1435.8578    1442.7432    1447.4134    1452.0173
1453.5802    1459.2478    1564.0888    1814.5674    2940.2998    2944.1681
2956.1554    2958.9778    2994.5143    2995.3570    3030.1919    3037.0132
3044.7675    3050.2335    3081.0035
```

```
==========================
        Structure  29
==========================
```

```
1312.8098i     49.6053      91.6508     119.6095     135.9191     166.2393
 202.6540     229.8462     250.9115     282.4389     342.4273     368.5417
 465.6240     488.6149     568.1969     702.8637     739.2474     786.1819
 817.3059     880.0568     931.6652     963.1975    1048.9108    1060.4412
1095.7266    1104.3306    1136.0983    1142.2719    1166.0738    1179.1066
1205.7163    1244.0306    1249.6895    1301.0325    1327.2117    1341.7838
1374.5522    1425.5888    1435.8224    1442.0636    1447.4714    1456.3474
1459.0770    1469.7424    1512.3741    1806.6852    2935.6240    2956.1090
2960.1928    2986.7557    2999.7370    3011.2493    3033.6775    3039.9630
```

```
3049.8687      3056.4186      3080.1964


                    ==========================
                         Structure   30
                    ==========================


1310.5882i      49.0251        64.4376        89.0481       122.4354       171.6762
 203.0229      222.6569       232.8975       298.6718       307.2818       362.7490
 422.6999      469.5250       568.3773       716.3476       733.2298       783.5984
 825.4791      877.8173       928.1549      1004.0875      1047.1202      1058.7138
1081.8810     1113.7478      1136.4604      1152.9123      1169.2758      1180.7613
1206.5461     1236.7428      1251.5628      1289.5621      1304.3361      1365.0677
1375.8740     1429.7343      1434.0018      1442.3430      1451.0285      1454.5828
1457.3528     1459.5265      1508.3531      1809.2511      2942.4293      2953.8321
2959.8224     2980.4869      2993.0220      3001.3737      3029.1471      3039.3529
3041.3006     3051.4306      3079.8208


                    ==========================
                         Structure   31
                    ==========================


1323.0167i      34.3792        66.4637       104.0153       128.4676       186.6514
 207.9182      223.1649       240.3041       258.6286       293.0051       368.0880
 405.4099      519.1105       546.0412       616.6867       732.6998       785.0113
 825.3876      878.1150       920.4704      1007.9788      1043.1193      1061.4003
1079.7852     1113.6698      1135.2071      1145.2478      1150.2414      1169.3362
1209.6599     1224.6201      1247.3663      1270.9101      1356.7971      1367.5767
1376.4231     1391.8410      1433.9776      1442.7616      1450.4761      1453.0043
1454.7651     1458.6281      1605.4817      1822.5581      2904.2762      2928.0052
2952.7760     2957.2202      2987.2673      3003.7085      3014.5731      3031.9229
3034.4026     3040.2818      3079.2871


                    ==========================
                         Structure   32
                    ==========================


1285.6589i      45.8816        89.9465       114.2458       135.4128       180.7495
 205.8382      216.4875       241.8349       314.6355       359.7485       410.7221
 433.0094      466.8672       563.0295       702.0919       750.1711       782.6753
 815.9964      889.3196       933.4923       951.5118      1035.0577      1068.6928
1091.1763     1109.3472      1134.5538      1139.2369      1166.9336      1189.6285
1202.3312     1238.4932      1260.9227      1296.3589      1320.6560      1357.6697
1366.5315     1428.5828      1439.3661      1444.6113      1447.7343      1456.1584
1460.7254     1464.4755      1558.9527      1806.4898      2953.3170      2960.6892
2965.5150     2971.2937      3004.8505      3018.1324      3031.9982      3036.7800
3045.4761     3049.9881      3081.3394


                    ==========================
```

```
                        Structure   33
                        =========================

   1316.0553i      34.2113      44.0674     109.1712     146.6984     191.5774
    200.2261      223.6888     236.9898     275.0398     287.6403     389.7375
    430.4414      521.1969     528.8978     602.1889     743.7628     789.8092
    819.8997      877.4523     926.6314     965.4646    1037.0430    1066.4269
   1080.8494     1111.8082    1135.0562    1144.8687    1147.9700    1167.0559
   1204.2768     1222.4917    1251.8580    1297.4795    1352.8892    1360.9363
   1368.0046     1393.5088    1442.5228    1443.4860    1451.1377    1453.4459
   1456.2354     1458.2501    1615.3585    1821.6234    2935.8511    2948.7869
   2957.0547     2970.7520    2985.7134    3007.7858    3017.3459    3031.7163
   3034.0126     3041.8100    3079.1790


                        =========================
                        Structure   34
                        =========================

   1299.8929i      37.0789      58.1081      98.3551     121.3627     172.1152
    207.0948      212.9275     239.2843     304.4313     355.9906     382.1178
    428.1429      468.6784     562.2007     720.2940     733.3279     779.7300
    820.3841      885.4352     925.9332     997.3146    1028.6089    1059.5479
   1092.3593     1112.9395    1137.5209    1142.5421    1167.9318    1192.7548
   1202.2077     1240.6440    1255.8425    1260.4129    1328.4212    1366.7481
   1377.8711     1427.9681    1431.1504    1443.6505    1450.8682    1454.7210
   1456.4915     1461.6032    1537.6666    1809.2736    2929.3778    2953.4226
   2960.6548     2969.0255    3000.6779    3013.6863    3030.6240    3041.3276
   3041.7867     3044.8798    3080.9540


                        =========================
                        Structure   35
                        =========================

   1322.4085i      38.3059      87.7686     109.9101     118.9499     168.0337
    191.7192      216.5574     260.6694     286.0025     311.1445     377.3182
    434.0293      468.9369     567.9263     698.9995     755.7477     777.6412
    822.3684      894.2393     929.0075     972.5419    1048.2056    1058.8377
   1089.4659     1114.8194    1136.4709    1153.1130    1171.6096    1187.2143
   1213.9808     1246.8627    1264.4965    1294.9062    1307.3272    1360.0529
   1370.4208     1431.0932    1432.6919    1441.7858    1448.2698    1456.0077
   1457.2192     1459.0074    1477.4725    1808.4518    2954.3114    2955.6009
   2962.5290     2990.9539    2997.6818    3009.0937    3031.4972    3043.3474
   3049.1483     3051.8817    3081.1123


                        =========================
                        Structure   36
                        =========================
```

1296.0474i	30.8409	74.0153	101.6276	151.4894	173.9828
189.9356	208.4219	248.5653	282.3679	311.0310	386.7238
442.7627	455.3639	567.5655	696.0276	759.6980	794.2624
822.4695	892.0427	930.6673	964.4899	1051.2719	1060.7152
1093.1713	1113.9789	1137.5353	1149.1196	1173.8191	1181.7061
1217.1109	1226.7134	1266.4759	1296.3961	1301.9097	1354.6988
1373.4616	1430.7535	1438.7651	1444.5354	1450.1371	1455.5894
1458.0240	1460.4500	1498.1064	1814.6680	2952.8349	2956.6616
2961.0597	2968.3386	2993.0710	3007.0658	3035.0504	3040.8356
3043.9762	3046.6845	3080.7854			

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==========================
       Structure  37
==========================
```

1357.1249i	44.0821	64.6693	105.4367	110.4938	161.8733
192.9559	220.7359	246.3382	307.0998	313.8458	348.8355
385.4311	462.2836	581.0238	701.7066	737.3639	793.6623
834.1763	894.4306	917.9224	1009.9020	1047.9030	1066.1750
1081.6069	1113.4703	1138.1069	1140.4415	1161.3137	1175.7364
1200.7657	1215.5189	1247.4471	1285.7424	1316.4839	1365.4226
1374.1796	1426.2668	1434.6553	1442.8927	1450.0592	1454.7606
1457.1242	1459.0490	1553.3502	1821.9239	2917.3821	2951.7258
2956.4701	2959.1546	2971.3731	3008.2511	3032.2530	3033.3973
3037.2718	3042.9200	3079.2006			

```
==========================
       Structure  38
==========================
```

1349.7503i	44.5088	67.9417	114.3952	135.0955	180.0692
198.4380	213.8479	239.2927	292.4331	316.9344	363.5449
427.1867	461.7244	576.5464	691.5663	748.7092	795.1880
840.1394	884.7455	933.1638	962.4783	1043.8952	1071.0409
1083.7614	1112.3145	1134.7688	1138.3606	1162.4385	1177.2754
1201.1565	1216.1812	1264.4899	1298.6890	1306.8670	1362.3542
1365.6607	1428.8400	1436.7566	1442.5894	1449.7553	1451.6469
1457.6687	1460.6400	1557.2344	1822.3777	2949.0057	2955.4805
2955.9855	2959.5829	2995.0608	3009.1812	3028.1488	3029.4397
3033.1986	3034.3972	3078.5213			

```
==========================
       Structure  39
==========================
```

1354.3344i	35.3741	69.3177	112.6170	129.5232	175.2988
193.8129	218.6788	238.3284	288.6902	323.6370	335.1747
461.2434	474.0114	580.9690	691.1362	740.2080	798.0908

844.3492	879.6377	918.2492	963.8117	1045.3508	1070.1270
1086.3989	1106.6813	1131.6108	1138.3967	1162.6877	1177.4856
1203.8991	1225.6796	1247.6279	1295.9477	1326.4290	1351.1874
1375.7980	1427.7727	1429.9615	1442.7363	1451.3370	1456.8522
1457.4512	1458.7151	1551.7273	1821.6240	2916.0410	2946.9225
2957.6956	2958.8093	2986.4964	3017.2921	3033.3952	3036.9065
3038.9728	3041.9585	3079.1037			

```
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        Structure   40
==========================
```

1354.5947i	37.3388	77.2210	86.3133	128.9920	161.9704
209.3281	221.6156	236.5272	298.1238	339.4674	358.8780
429.0435	467.7187	561.7227	703.3137	742.5283	786.2102
817.7768	882.9156	920.2400	989.8681	1044.7806	1052.2090
1091.5429	1108.0948	1136.6526	1137.6263	1160.7898	1180.5327
1195.6376	1242.1907	1256.5102	1267.2475	1325.6258	1363.5514
1374.0126	1427.5684	1433.1750	1442.5430	1449.8004	1454.9403
1457.8675	1460.8339	1588.8450	1817.6823	2905.6013	2957.1896
2959.5446	2968.8754	2973.0444	3017.1443	3029.1087	3034.3335
3041.9964	3044.9129	3077.9621			

```
==========================
        Structure   41
==========================
```

1360.0487i	57.1739	85.1879	115.0909	161.4381	185.6455
202.0647	222.5237	264.6222	306.3129	369.8309	384.5460
454.5619	489.3709	561.1872	699.1576	750.4046	791.0249
817.8868	886.9127	927.8930	961.3829	1041.6881	1068.4279
1087.9920	1109.3271	1137.1060	1145.1766	1178.2235	1183.5477
1222.7349	1242.2674	1258.1867	1296.7498	1325.0135	1330.2332
1383.2599	1425.8447	1431.2155	1443.4995	1451.2509	1453.5148
1455.5670	1459.7139	1490.0195	1814.8351	2919.6038	2960.5002
2961.3162	2981.9623	2985.6284	3018.9719	3038.6868	3038.8481
3042.4267	3049.3617	3081.2924			

```
==========================
        Structure   42
==========================
```

1337.0020i	40.5906	90.3512	99.7914	130.1408	200.0707
215.9418	223.9113	257.4719	299.2626	321.4213	359.0937
450.2818	515.5989	555.5238	602.0571	740.4287	778.7718
824.9732	875.6378	920.0328	974.0375	1041.1331	1069.8180
1080.9199	1099.9221	1135.1398	1141.2517	1147.8991	1169.5673
1203.1591	1224.3071	1250.7907	1327.0914	1335.1373	1352.2579

```
1379.8922     1394.2044     1427.3375     1441.9850     1447.3015     1453.1195
1453.3143     1459.3509     1646.0107     1827.4230     2905.4509     2927.3645
2956.4241     2958.6751     2981.3182     2987.0585     3024.7671     3029.9796
3033.5944     3055.9581     3077.5242
```

```
==========================
       Structure   43
==========================
```

```
1286.7159i      22.4202       97.7300      123.6994      127.1159      165.6231
 194.1640      226.2108      286.2236      296.5292      346.7272      362.3903
 458.8974      490.9344      562.0543      697.3691      761.2393      773.4142
 816.8835      891.1958      922.3878      961.4830     1041.6709     1070.2605
1085.9959     1106.6324     1137.9838     1140.7289     1164.4066     1179.0947
1222.3840     1246.0859     1270.2238     1294.5109     1321.1255     1354.6501
1376.6673     1427.7341     1429.7252     1445.1928     1452.4927     1455.7986
1458.5491     1460.5167     1553.4921     1806.8386     2943.3465     2961.4476
2963.6542     2972.7529     3000.0044     3022.1214     3024.2911     3039.5482
3046.6788     3054.2678     3081.7443
```

S.3.5 $(\mathbf{TS}_\gamma)^\ddagger$

```
==========================
       Structure    1
==========================
```

```
1260.5365i      36.7298       64.9666       94.5462      137.0309      168.1441
 189.4699      204.5872      238.1479      289.5526      316.0734      329.7603
 357.0336      509.0859      572.5726      642.9353      779.4847      827.5406
 837.4953      905.5735      931.6276      998.7730     1032.1613     1060.8198
1080.3320     1110.5785     1145.8316     1151.4564     1174.2813     1192.4629
1204.8761     1229.5017     1245.6261     1282.5478     1359.1443     1373.1140
1381.0038     1411.4644     1418.6393     1437.8428     1439.2373     1441.3054
1443.6366     1454.5685     1541.6290     1794.2997     2940.0970     2944.4885
2974.5722     2981.7562     2992.6517     3009.0808     3022.5639     3031.4067
3044.2487     3064.9893     3098.1514
```

```
==========================
       Structure    2
==========================
```

```
1287.2361i      29.5595       61.2951      101.2013      107.2320      135.5803
 171.6769      192.2240      241.9456      277.7155      322.6282      335.3721
 343.3012      475.0873      568.5678      688.7986      740.0742      810.2386
 880.1010      911.1283      921.7603     1012.1218     1035.8327     1069.8997
1085.9597     1107.3721     1146.0083     1150.8265     1172.7576     1196.5731
```

1203.3669	1211.8814	1263.3643	1268.8000	1342.9023	1372.6756
1391.3499	1414.0310	1429.2267	1438.5926	1439.9285	1441.0184
1444.1708	1454.9195	1528.1881	1797.7674	2940.8401	2944.7715
2971.0050	2981.3274	2991.5981	3004.8712	3013.4871	3018.7065
3043.0960	3064.4373	3097.3962			

==========================

Structure   3

==========================

1279.8611i	32.5613	47.0055	102.9817	137.3243	165.7200
177.3080	210.8883	244.7615	285.8598	317.6139	361.1674
384.6066	493.9403	573.4339	646.6538	786.5326	821.7057
843.3950	903.0114	931.8983	976.8198	1030.4000	1039.0196
1079.9854	1114.0525	1145.9623	1161.8093	1172.8497	1183.4504
1197.4124	1227.1379	1245.1647	1307.6153	1348.4798	1370.6635
1374.4219	1412.1513	1426.5349	1437.5717	1438.7050	1441.1422
1447.2212	1454.6054	1545.1899	1796.4387	2938.4034	2963.0808
2973.9418	2981.8962	3004.7429	3015.7298	3028.4868	3033.5151
3046.8485	3065.3039	3098.2424			

==========================

Structure   4

==========================

1271.0586i	33.8362	88.1778	105.7397	139.7601	170.6314
210.0004	240.5588	255.2985	296.0201	302.8648	342.2103
397.6251	514.1894	571.6008	657.2342	799.7735	807.6525
846.9923	913.6666	926.5923	966.1349	1031.5158	1053.6035
1081.5731	1107.8107	1146.0022	1150.7009	1173.8084	1193.5341
1210.3423	1216.5055	1246.2273	1330.3384	1335.3870	1371.8904
1376.2411	1413.4374	1420.9340	1437.3357	1440.2415	1441.6713
1448.2191	1454.4333	1522.5593	1794.1935	2945.1625	2952.2364
2972.2416	2981.7998	3005.5805	3012.3345	3023.6216	3025.6363
3040.3437	3065.2020	3098.2336			

==========================

Structure   5

==========================

1284.2526i	27.6158	58.0130	97.4780	131.2487	134.8273
170.7106	201.7599	226.0600	293.6869	304.8432	328.6951
412.5810	474.5644	571.2808	695.4204	743.9537	807.7460
866.6562	908.1519	928.6577	968.4993	1036.1537	1061.1128
1099.9836	1102.6871	1142.9571	1146.3501	1172.8228	1190.3198
1204.1878	1212.5381	1267.8215	1304.4578	1327.5896	1372.8327
1384.6572	1414.6488	1428.7524	1439.0023	1440.8373	1442.0148
1446.4831	1454.8782	1536.8829	1797.6229	2937.8280	2941.2012

```
2973.6983     2981.3236     3005.2105     3011.4698     3023.1101     3025.5833
3045.3734     3064.4204     3097.3637
```

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                        ==========================
                           Structure    6
                        ==========================
```

```
1290.2355i      25.5738       58.5670       90.3651      119.3997      135.8677
 172.3919      193.8854      229.8097      278.0615      311.3760      355.5170
 400.5419      449.0306      569.2741      690.0501      749.9533      812.1177
 867.6262      905.2875      923.8644      985.9014     1027.3074     1068.7063
1091.1834     1094.0913     1146.0542     1171.0511     1174.7733     1184.4576
1203.8019     1207.9387     1269.2139     1285.6150     1338.4995     1369.6992
1381.3083     1412.3877     1433.5939     1437.8345     1441.0711     1442.0076
1446.0431     1454.8970     1547.4328     1799.2375     2940.0993     2968.8212
2976.2165     2981.6334     3001.8246     3007.5309     3013.6870     3030.2098
3040.1074     3064.9459     3097.6496
```

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                           Structure    7
                        ==========================
```

```
1296.8820i      34.1576       80.5108       92.5176      141.6413      174.4447
 194.1326      204.3268      250.8395      291.7247      338.3873      369.5893
 396.8929      473.3925      600.4951      677.6146      792.0546      825.4127
 841.4109      882.5396      928.6862      995.1403     1034.0042     1050.3171
1085.1265     1102.6995     1145.6111     1168.4347     1176.9756     1192.4931
1200.0921     1210.0235     1262.8924     1297.6654     1336.3381     1361.2504
1378.4441     1421.9032     1425.8181     1436.6406     1439.9445     1440.6751
1443.6430     1451.8953     1536.6005     1800.9342     2931.0293     2941.2067
2979.9496     2983.7047     2994.6616     3008.5726     3017.2001     3043.7522
3050.2521     3064.1185     3096.3458
```

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                           Structure    8
                        ==========================
```

```
1301.6843i      17.6344       55.4529       91.0164      140.5437      174.8830
 193.1040      212.7548      250.1785      294.8851      326.7307      356.0366
 374.5740      485.5849      580.7094      672.6559      783.9470      822.1400
 845.8173      910.5964      926.7190     1001.4860     1027.2343     1045.8272
1085.9886     1097.8242     1145.6638     1169.4479     1176.1351     1191.5889
1207.8324     1216.2964     1251.8553     1279.2679     1353.9259     1368.6535
1380.4398     1420.1610     1425.2777     1438.0455     1440.0715     1440.3093
1443.0188     1453.1096     1547.9607     1796.8852     2933.3882     2939.1774
2975.9172     2981.2539     2997.1366     3009.2184     3013.4664     3035.7626
3043.9834     3065.3756     3097.7006
```

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==========================
        Structure    9
==========================


 1287.1881i     31.7079      63.8458      77.1216     138.0284     177.0266
  186.1531     201.0413     243.9830     296.7384     316.7869     332.8403
  373.1371     513.5998     585.4510     638.4456     783.0556     827.1664
  840.0434     873.6006     931.0007     989.7393    1046.6092    1062.7607
 1085.3256    1106.0540    1146.3693    1152.0251    1175.7173    1190.2128
 1201.7217    1228.8019    1266.1432    1299.7599    1335.2431    1360.4752
 1380.5262    1416.3695    1423.7992    1435.2327    1439.9167    1440.2192
 1443.5512    1454.5369    1540.6837    1799.4026    2940.4308    2947.6493
 2974.8825    2981.6853    2990.2866    3007.4358    3015.9974    3042.4431
 3042.8103    3065.2546    3096.9050


==========================
        Structure   10
==========================


 1289.3960i     57.8831      80.4101     129.9693     147.1859     161.3674
  191.2420     229.4763     293.0408     305.4366     316.1628     360.3790
  417.4081     508.6389     602.9793     692.2634     789.7085     815.0645
  843.7397     890.1586     929.6473     967.9237    1013.5955    1056.1526
 1087.7661    1103.7926    1145.6173    1149.5656    1173.0684    1178.7511
 1211.0411    1220.3095    1279.0794    1315.9754    1337.9467    1349.8005
 1375.4881    1420.7495    1426.8788    1438.1849    1440.3002    1442.5954
 1452.1193    1454.9635    1535.6814    1796.4153    2933.8490    2935.4479
 2980.3206    2993.0624    3003.3761    3013.6267    3019.7127    3048.8963
 3059.0271    3064.8129    3097.0457


==========================
        Structure   11
==========================


 1289.8738i     27.6511      62.8320      99.9372     138.7830     167.8266
  209.8668     227.9312     240.5981     287.1014     305.8417     367.8274
  379.5161     489.8108     570.2053     663.8471     797.1152     813.5651
  845.8260     912.2130     918.1564     982.7162    1025.5756    1042.8445
 1087.8490    1104.8176    1146.0688    1161.7507    1173.5225    1195.8725
 1205.6369    1219.6114    1249.1596    1305.1657    1347.7564    1367.5015
 1379.2765    1414.3268    1428.1085    1435.0303    1437.4322    1440.9129
 1446.7407    1454.3432    1537.1626    1796.3868    2938.3006    2965.3273
 2973.7894    2981.9598    2999.3774    3010.4589    3021.7671    3030.1194
 3049.5843    3065.5056    3098.4402


==========================
        Structure   12
==========================
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```
  1293.7738i      23.5226      65.9266      92.9909     108.2972     139.5875
   182.0782      193.4524     241.5488     286.8483     320.9682     334.8161
   361.4428      444.0812     625.7893     699.0800     742.3142     810.0422
   865.8411      890.3437     927.6054    1017.8283    1043.8191    1063.5596
  1088.0677     1108.7371    1146.3140    1152.1634    1176.0897    1196.9620
  1209.8099     1226.7832    1259.1576    1300.5031    1323.8133    1365.0112
  1378.9674     1422.2884    1433.8918    1435.6495    1440.1053    1440.6289
  1443.9506     1454.4754    1531.7071    1799.1365    2925.5575    2940.9905
  2972.5789     2981.6524    2999.0871    3008.4951    3015.4649    3043.2829
  3046.0254     3065.1149    3097.2128
```

==========================
        Structure   13
==========================

```
  1298.3368i      19.9103      65.2955      92.6329     108.3265     139.0156
   185.1830      191.4678     234.7416     292.3731     322.7843     332.2858
   361.8766      442.3297     624.2790     692.8565     747.9004     807.9566
   865.6593      892.6244     924.3429    1011.2383    1045.0362    1077.2167
  1085.6014     1102.4538    1146.2522    1153.1567    1175.6113    1196.7248
  1210.3343     1223.8807    1262.5802    1297.7713    1322.4678    1365.2065
  1380.1543     1422.2031    1433.7441    1435.3364    1440.0996    1440.4372
  1443.9437     1454.4899    1534.3957    1800.4218    2940.4563    2945.3854
  2966.2542     2981.6257    2985.9800    3005.6363    3013.9054    3043.0170
  3049.7588     3065.2158    3096.8830
```

==========================
        Structure   14
==========================

```
  1281.3494i      16.9635      53.5520      90.9758     136.2535     153.9539
   173.3704      216.3416     264.4145     290.2366     305.2394     366.4609
   410.7379      465.9310     604.4230     693.8954     790.4508     821.7389
   843.6246      886.5363     928.5745     971.4025    1033.8422    1035.1673
  1093.2835     1104.5884    1146.0633    1151.7287    1175.3816    1180.9356
  1195.2205     1219.6931    1273.7248    1315.4165    1321.7357    1356.2150
  1373.8734     1424.8361    1430.3740    1435.9041    1440.6698    1443.4203
  1451.9323     1454.5881    1551.9389    1796.2912    2941.9888    2965.7029
  2981.3973     2989.1851    3004.6719    3014.2435    3024.9718    3039.4788
  3059.4479     3064.6160    3097.9291
```

==========================
        Structure   15
==========================

```
  1296.3412i      49.8822      83.3921     132.1386     144.7927     159.2430
   205.3606      230.5260     293.3563     299.9160     313.0455     360.7828
```

417.4299	497.5106	607.1031	711.4202	788.7719	815.6162
846.2282	891.3243	942.8588	960.9791	1024.7876	1038.9002
1090.5089	1099.5873	1145.4905	1150.4487	1168.5982	1179.2108
1210.9229	1215.7655	1260.4650	1327.4332	1335.1231	1353.3241
1372.7093	1422.5764	1426.5702	1439.5008	1439.7554	1442.8915
1451.4243	1457.5681	1541.9334	1798.7228	2932.8836	2936.4627
2981.0207	2997.9781	3006.1812	3015.0772	3020.7724	3049.0619
3058.1435	3065.9081	3097.5475			

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==========================
      Structure   16
==========================
```

1290.6800i	52.3459	59.9855	80.7679	140.1108	169.8281
200.5695	236.6810	244.4469	291.4916	305.1822	373.5985
397.5109	479.1115	593.1043	671.3358	805.7269	809.5728
842.9171	883.3370	919.4653	984.3779	1025.0391	1041.7103
1098.5837	1103.7059	1145.7785	1165.7781	1176.0368	1200.0356
1207.5785	1221.1851	1275.1435	1306.1027	1339.0033	1354.3652
1376.4667	1420.2200	1429.5630	1431.7328	1440.1605	1441.3596
1450.7790	1455.4822	1519.9319	1796.1553	2941.8176	2966.9282
2975.2954	2978.6990	3003.5514	3013.0945	3021.9366	3039.3508
3048.0785	3061.5969	3096.8873			

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==========================
      Structure   17
==========================
```

1293.9282i	22.8529	53.7342	93.1806	107.2113	138.2605
183.7056	203.0850	231.1791	282.5264	303.4010	360.5844
403.8936	431.8572	630.6065	716.3185	747.0859	811.2131
865.9398	877.1168	932.3561	983.1215	1040.0485	1049.9303
1092.4762	1103.2175	1146.1938	1174.3710	1175.5695	1185.2493
1204.1378	1234.3484	1271.0226	1302.9446	1328.5899	1349.9840
1375.2245	1423.3119	1434.1576	1437.8257	1440.5639	1444.8022
1447.6620	1454.5479	1539.7573	1798.9630	2941.5945	2964.4574
2981.0340	2981.8109	3004.3609	3011.4859	3021.1873	3041.2222
3052.3413	3065.2506	3097.6167			

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==========================
      Structure   18
==========================
```

1292.4605i	21.9638	52.7908	90.0281	110.1753	138.9018
184.4033	204.2223	223.6951	285.6727	304.9695	367.3890
404.6716	421.1659	631.1282	709.8604	758.3045	813.3185
867.6824	875.4867	926.6782	983.1514	1035.9848	1055.1937
1092.8773	1103.3158	1146.2996	1172.1750	1176.8649	1184.8237

1204.2436	1238.2010	1265.0539	1308.4165	1324.2178	1352.1128
1376.3229	1423.6056	1434.5758	1437.5801	1440.6684	1444.4799
1447.7980	1454.6056	1539.7857	1799.1293	2942.8333	2959.1938
2977.3801	2981.7564	3004.3420	3012.7936	3022.6873	3041.3640
3058.5984	3065.1963	3097.7171			

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Structure 19
==========================

1291.0840i	23.2462	51.8891	97.5316	122.7147	139.1388
193.4848	203.7178	224.5897	290.5747	302.8686	329.5775
423.3715	459.4661	625.2681	701.6329	752.0996	809.5027
865.8261	875.2756	931.5090	971.7523	1037.8068	1070.5330
1097.4357	1101.6095	1144.8825	1146.3574	1176.1681	1189.9406
1204.7854	1247.4944	1265.6849	1305.6356	1332.5077	1357.8154
1374.3502	1422.8244	1434.0131	1437.3058	1440.3471	1442.1470
1446.7013	1454.5088	1539.5870	1798.5914	2923.9264	2939.3121
2972.5894	2981.5275	3011.8049	3015.7073	3024.2612	3046.2185
3058.9594	3064.9454	3097.1794			

==========================
Structure 20
==========================

1288.1424i	47.2408	70.1997	90.5248	139.5765	175.9951
202.8226	232.5749	247.7247	294.7379	302.3029	341.6746
414.3597	519.9186	578.1310	650.9752	803.1451	804.8633
846.3215	879.2282	922.5034	967.2659	1030.2426	1068.4189
1081.4464	1107.6365	1145.9403	1151.4987	1175.9047	1194.7663
1209.2696	1219.5693	1279.1836	1330.8549	1335.9679	1344.6598
1375.2613	1415.0471	1423.9971	1434.4588	1440.0491	1443.2102
1451.9124	1454.5707	1529.2251	1795.6443	2941.0729	2953.4562
2972.2373	2980.9940	3001.1537	3012.8524	3020.7715	3039.6579
3043.2180	3064.5471	3096.4585			

==========================
Structure 21
==========================

1248.4047i	46.2825	68.0400	106.6789	128.2285	191.3366
194.4915	226.5004	246.6357	275.4617	317.0660	331.4562
410.0350	529.2638	549.4076	584.3985	750.5412	806.9135
833.3842	883.5259	932.0848	1008.2300	1055.1597	1075.7482
1086.5832	1112.6707	1137.4708	1144.8560	1157.2583	1196.6954
1206.4853	1228.0972	1245.7363	1284.6099	1359.5325	1370.5469
1380.7883	1405.9906	1417.4587	1438.8921	1443.6441	1445.1333
1455.1891	1460.5317	1538.9689	1815.6887	2941.2077	2949.0705

```
2959.9801      2964.1511      2994.3454      3009.9178      3010.3286      3035.4404
3040.4679      3047.5407      3083.7692


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                           Structure  22
                       ==========================


1281.2200i       38.9107        75.8298        98.3786       107.5896       126.7267
 191.4067       197.6699       244.9156       273.6576       324.0033       337.3055
 396.9596       525.5674       534.5566       587.0872       744.9025       812.0382
 839.0437       896.2639       921.8197      1023.4691      1063.3302      1082.6260
1087.2081      1107.1041      1136.5383      1143.1005      1154.6820      1198.3116
1206.4550      1213.3722      1261.6573      1273.1396      1341.4688      1372.7644
1389.1261      1408.6063      1428.4568      1439.3442      1443.6453      1444.8914
1455.2429      1459.2978      1526.5997      1819.1527      2942.2625      2950.7391
2956.5568      2962.6060      2992.6192      3001.1939      3012.2405      3015.6160
3039.1009      3044.1420      3083.6990


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                           Structure  23
                       ==========================


1278.8902i       34.1389        74.9868        93.5708       116.7567       136.8797
 193.8825       206.0835       244.3339       296.3808       299.2449       331.1037
 471.0177       505.5398       536.1748       593.3810       748.5361       808.5635
 843.5031       879.5590       929.3824       977.1224      1055.9486      1084.1946
1101.6902      1103.2000      1136.5325      1140.6284      1147.8384      1191.3773
1203.6294      1214.8343      1274.2435      1300.2919      1327.7333      1372.7410
1381.8909      1409.1956      1427.9833      1441.6959      1444.2942      1446.2772
1455.4810      1459.6583      1536.5204      1818.9956      2938.7585      2949.0183
2959.1776      2964.1097      3000.2945      3010.5543      3020.6650      3027.5022
3038.7143      3045.0211      3083.5737


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                           Structure  24
                       ==========================


1281.0800i       42.2366        46.1120       110.5256       128.4452       188.2149
 193.5745       223.6345       243.6087       278.0027       315.4369       371.2459
 419.2943       525.5226       541.8905       585.6559       754.0338       814.0132
 828.3490       883.3190       930.4086       986.5689      1035.1367      1071.3355
1087.7699      1114.9796      1136.9524      1147.5534      1164.2339      1187.3386
1196.2068      1224.8991      1246.9002      1309.0847      1349.0420      1368.2177
1374.5975      1405.8572      1425.7301      1437.6726      1444.5675      1447.3114
1455.1225      1459.9684      1544.3560      1817.7193      2936.0073      2956.4242
2961.2967      2966.4697      3001.8670      3006.0964      3026.9938      3035.2494
3038.5446      3055.0963      3083.5074
```

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        Structure   25
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 1255.0108i     46.6560      97.9962     109.7173     137.9193     198.9054
  226.0072     246.1422     253.3345     295.4960     301.1125     343.7970
  451.9709     528.2947     555.6001     576.0657     759.4342     805.9805
  828.7938     894.5187     926.8566     975.6789    1049.3535    1072.5959
 1092.4182    1110.8706    1137.0965    1143.3631    1158.2555    1200.0456
 1211.1315    1217.0199    1244.6659    1331.5920    1336.4095    1369.7889
 1377.1381    1406.3180    1419.6383    1437.0511    1443.7927    1445.0217
 1455.2199    1461.0438    1515.6441    1815.8317    2951.0093    2958.4301
 2960.3721    2963.5295    3007.0342    3010.7996    3016.9457    3027.2347
 3040.5711    3042.0196    3083.5625


==========================
        Structure   26
==========================


 1295.4979i     31.3840      75.8476      91.0791     117.1985     126.9054
  194.0247     203.4895     247.5277     265.7550     313.5913     369.9815
  422.9391     510.0576     533.3474     588.6250     754.1239     812.5868
  839.9519     877.8754     924.6370     993.5920    1054.2675    1082.9682
 1092.0356    1096.3261    1136.8386    1144.8377    1173.9212    1184.5006
 1203.4532    1210.8187    1272.0247    1284.3284    1337.5503    1368.2653
 1379.6841    1406.4870    1433.9573    1440.7173    1444.5397    1446.0081
 1455.4109    1460.0975    1545.3498    1820.7491    2938.3253    2955.3861
 2961.8447    2980.0240    2998.3343    3001.9913    3010.6624    3032.9080
 3037.6125    3040.9573    3083.4413


==========================
        Structure   27
==========================


 1290.7747i     39.8467      69.8132     103.5377     134.4122     202.5188
  215.4385     229.2919     251.3625     277.4715     307.0669     368.8400
  421.5120     527.4894     540.4936     576.5533     760.0302     809.8764
  824.0359     889.7957     919.6575     999.3481    1031.0857    1075.9054
 1093.6228    1107.1037    1137.3702    1146.8913    1166.8777    1200.9593
 1209.3309    1218.1791    1247.4668    1307.2006    1348.8091    1368.3080
 1381.7795    1405.2317    1426.5124    1433.2884    1442.5555    1444.6540
 1455.4506    1461.3379    1531.6202    1819.1477    2943.0934    2953.7770
 2961.1946    2974.0943    2993.5116    3005.1708    3013.1960    3030.3876
 3038.9842    3053.7451    3083.0679


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        Structure   28
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```

1271.1032i	45.3555	68.7206	113.2992	115.5126	166.7832
192.7196	206.8569	250.0209	316.3699	324.8221	342.4577
380.5983	469.7000	583.2044	707.2056	738.4071	804.7455
833.1525	893.2322	931.0505	1008.3617	1044.7296	1069.9612
1094.9403	1114.2187	1134.3379	1138.8701	1164.4042	1196.8418
1203.7922	1221.9468	1248.5505	1289.3008	1324.1048	1362.3416
1377.8130	1431.6049	1439.3434	1442.6201	1443.5057	1447.7720
1461.4695	1464.4850	1526.1649	1817.2049	2939.9546	2944.1657
2961.9082	2978.6773	2997.7562	3009.9386	3018.0307	3040.9661
3045.2083	3056.1795	3082.6107			

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Structure 29

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1321.0290i	44.6528	46.9006	94.7905	132.4011	190.6258
204.7094	236.1978	251.5730	289.6454	316.7449	366.1250
411.2676	527.0787	547.8220	581.9860	750.8353	806.1370
830.1153	886.1099	930.7288	1021.6081	1027.0167	1080.7253
1087.4114	1101.0346	1137.5484	1147.2209	1175.9412	1201.5503
1215.5478	1217.2097	1240.7944	1282.5785	1351.5250	1368.8185
1383.3129	1408.1541	1424.2517	1440.0102	1442.7482	1444.1295
1455.5103	1461.6784	1554.2806	1820.9780	2934.3118	2938.1138
2959.0935	2962.9281	2992.7443	3009.6361	3011.7365	3024.8343
3038.0049	3045.0769	3081.8733			

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Structure 30

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1276.2340i	51.4348	87.8860	121.6525	122.9660	168.0228
197.9409	214.8997	252.5006	297.1459	329.3784	365.5996
443.1641	477.8095	563.2004	709.5327	739.3098	810.4592
820.1433	889.3143	929.5839	969.7545	1034.9544	1056.9989
1100.3676	1108.5028	1137.1884	1139.6668	1167.7863	1186.1419
1196.9121	1217.1037	1266.4470	1308.6271	1321.8373	1357.7687
1374.3424	1430.3831	1435.2905	1444.5887	1445.4069	1452.7240
1460.6700	1463.4696	1552.3860	1810.9223	2944.5453	2958.3777
2964.0770	2997.9405	3006.9624	3015.9093	3030.7059	3041.5376
3043.9440	3057.5770	3083.5549			

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Structure 31

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1293.9817i	41.4259	54.3044	126.2387	150.8305	206.1335
214.3065	217.4761	268.9097	326.1178	357.7189	374.3237

431.0709	533.9684	548.8601	581.0990	750.5463	804.9427
823.0799	894.6956	944.0148	1001.1634	1034.2447	1072.3703
1088.1924	1107.6937	1137.5569	1148.7578	1184.9484	1190.7507
1218.3057	1234.1677	1251.7880	1295.4757	1345.7525	1367.0542
1371.7023	1406.9625	1428.8196	1437.5754	1444.1475	1446.3618
1455.6214	1461.4191	1502.3209	1813.7926	2938.0179	2958.5309
2961.0694	2967.8789	3005.3403	3013.8280	3015.5482	3027.4285
3038.8113	3053.0608	3082.9293			

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==========================
      Structure  32
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```

1268.1107i	50.6983	65.5699	118.0515	133.2417	172.8122
204.7462	217.8067	226.2569	300.2554	328.2148	338.9968
464.5266	473.1383	586.7801	698.0802	740.6572	809.1089
839.1826	877.9572	931.1835	961.1690	1043.6446	1076.1448
1103.6905	1104.4939	1126.6844	1138.3883	1164.7692	1190.5122
1204.6396	1232.8108	1257.1216	1302.4371	1330.6208	1350.1420
1374.7364	1429.6080	1440.1417	1441.9663	1447.2604	1448.4651
1461.8859	1464.9385	1528.5789	1816.8652	2941.0187	2944.9775
2961.9522	2988.4914	2994.8981	3013.9729	3025.8409	3041.2218
3048.0080	3060.8958	3082.7214			

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==========================
      Structure  33
==========================
```

1287.6383i	53.0568	68.5928	99.1603	126.6677	183.7701
191.5066	201.9191	242.4257	306.9684	321.0776	331.4000
422.8733	471.7758	561.5854	711.1996	745.5643	808.9505
827.7107	886.1216	933.6242	993.5909	1042.9460	1071.3914
1092.9639	1109.5048	1133.7902	1140.4177	1163.8884	1187.3334
1195.7374	1218.5107	1258.8822	1291.8417	1325.2197	1361.6015
1382.1066	1427.6287	1439.6249	1443.2321	1443.4800	1444.5941
1459.8132	1462.0883	1532.8053	1813.4207	2922.7650	2939.6929
2961.9984	2979.3263	3003.5653	3007.5251	3037.4677	3041.0961
3048.8756	3057.5195	3081.8275			

```
==========================
      Structure  34
==========================
```

1314.4098i	45.8944	62.5459	105.5620	118.1309	151.1208
190.9078	206.2805	239.6273	316.0413	326.1916	331.7499
381.6253	469.2035	583.0649	704.8627	734.3945	805.7337
828.8044	897.9831	924.3728	1004.4282	1041.3189	1074.5643
1090.4708	1114.4559	1137.6860	1142.7984	1164.8939	1194.4107

```
1208.2499     1218.5703     1252.0446     1289.6769     1323.6398     1361.8373
1376.5329     1431.1431     1439.8431     1442.7114     1443.2704     1446.4343
1460.2703     1463.5207     1536.7445     1818.7398     2918.9072     2941.3697
2960.0484     2990.1963     2997.2612     3007.2264     3014.8630     3038.1386
3045.2399     3056.5420     3081.1047
```

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==========================
        Structure   35
==========================
```

```
1304.6466i      46.7379       66.7565       85.3813      130.2276      188.8128
 206.9216      231.4462      244.5087      300.9507      357.7235      373.7432
 442.8714      528.5504      546.6028      575.7982      762.1165      799.6096
 835.6507      895.5628      936.0678      978.0771     1022.8353     1079.5486
1082.8945     1102.4867     1137.5684     1146.6484     1159.7937     1186.7542
1204.1007     1222.2317     1241.4716     1316.9632     1332.7117     1370.4196
1373.8421     1406.3207     1423.8878     1438.1502     1443.6226     1445.9547
1455.7961     1461.7591     1547.1641     1820.5023     2937.1846     2940.0497
2959.3978     2965.3640     3005.3271     3012.9152     3032.5848     3037.9226
3039.9587     3048.1651     3082.0017
```

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==========================
        Structure   36
==========================
```

```
1307.2667i      45.7880       55.1739      102.8854      127.6819      156.5428
 194.0147      204.5735      222.9058      295.4201      325.0186      370.6287
 408.6766      470.8038      582.3341      698.9018      740.5046      812.4142
 833.1320      879.5604      925.4052      975.9120     1037.3909     1061.6694
1091.9034     1116.8008     1138.4587     1153.2574     1174.2384     1186.2365
1205.4393     1230.9383     1256.0260     1306.2525     1322.2668     1348.6030
1376.3780     1432.4337     1440.5171     1442.9586     1445.2957     1448.5090
1460.1572     1463.6914     1534.8282     1816.2827     2943.8436     2959.6661
2962.1842     2996.6856     3000.6689     3011.9578     3017.9896     3039.9108
3043.6084     3059.4907     3082.2371
```

```
==========================
        Structure   37
==========================
```

```
1308.8301i      40.5344       54.5238      102.4284      129.0319      158.7917
 196.1921      204.7482      226.5408      296.7556      319.7290      362.8803
 414.2539      470.4214      582.6909      698.5449      743.7217      808.2785
 829.0577      881.1120      930.4119      975.2907     1038.7876     1060.1520
1092.0760     1116.2429     1138.3220     1153.3907     1175.2276     1183.8994
1202.3196     1227.8616     1263.0620     1295.6858     1327.4835     1347.7400
1375.1013     1432.4853     1440.2452     1442.6371     1446.4779     1447.9661
1460.4237     1463.5210     1538.6342     1816.6211     2940.1460     2955.6737
```

```
2961.3140     2999.5981     3005.1219     3011.3537     3021.7883     3039.6630
3040.9665     3057.4987     3082.1840


                    ==========================
                        Structure  38
                    ==========================


1313.5335i      37.5242       55.0972      104.3620      133.4941      166.9840
 203.7430      209.8564      218.1147      296.5298      317.7198      335.8386
 462.9264      470.1542      586.5320      694.6404      735.9207      805.8580
 828.3149      883.4982      934.0172      957.8687     1043.5003     1080.7295
1099.3429     1104.5382     1133.3569     1139.4282     1164.6630     1188.2658
1202.9065     1230.3171     1262.9274     1303.8690     1326.9348     1350.9238
1373.6177     1427.7489     1440.8870     1442.9313     1445.7830     1448.6484
1460.9465     1464.3598     1546.1644     1818.5512     2917.9831     2936.2617
2959.7829     3000.4224     3007.6433     3011.3188     3026.4277     3037.9136
3046.3880     3059.4674     3081.0718


                    ==========================
                        Structure  39
                    ==========================


1321.0890i      55.6038       78.9653      108.9129      121.2646      180.8549
 189.3074      201.6057      248.3386      313.9029      319.6920      345.2368
 427.9863      469.3850      561.6262      704.1012      744.3141      805.4420
 825.4558      898.3247      929.1248      997.8754     1040.3029     1058.9618
1084.9831     1118.5949     1137.4531     1149.9102     1168.5823     1188.9322
1193.9904     1210.0755     1259.8934     1294.9189     1327.1482     1362.6803
1380.2689     1427.0514     1438.8810     1443.2839     1443.8594     1445.2493
1457.6984     1461.5183     1526.6459     1814.1910     2934.0135     2940.3296
2963.4255     2972.0819     2997.9735     3007.4119     3032.6513     3044.3931
3045.5908     3053.6316     3082.8823


                    ==========================
                        Structure  40
                    ==========================


1285.8282i      41.2085       66.1003      115.4391      122.6894      179.2986
 193.0594      194.5345      256.8530      305.0149      321.0235      362.7767
 429.6553      471.6454      561.6817      703.7540      744.7430      803.1268
 818.2795      899.7361      927.9641      978.2036     1031.0083     1053.6880
1096.0449     1117.7059     1138.3865     1152.1292     1176.5384     1196.7001
1202.6692     1217.5036     1267.4742     1295.8456     1332.7501     1360.1185
1377.2012     1430.7061     1433.9748     1444.1456     1445.1310     1449.8123
1459.5016     1461.8367     1504.9746     1811.6806     2950.7993     2955.3727
2965.3583     2992.3101     3001.3870     3018.4381     3027.8233     3040.2417
3045.9902     3054.5527     3083.9554
```

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==========================
        Structure   41
==========================


  1286.5412i      45.5205      91.4524     100.5382     150.0868     189.5531
   197.8731      212.5787     226.3411     293.8269     322.1495     335.0516
   456.5487      484.5609     562.3801     698.0965     756.4129     806.4077
   815.2126      896.0994     931.8819     958.3122    1039.4603    1074.5292
  1088.6801     1114.6169    1135.7354    1143.4936    1165.6046    1182.7451
  1208.3313     1213.5597    1265.3344    1320.8993    1329.5519    1334.0513
  1381.3535     1430.5337    1436.5793    1441.2562    1444.6033    1450.2528
  1460.5632     1462.0582    1534.0142    1817.8982    2927.1817    2941.6747
  2963.3874     2991.3126    3003.5285    3017.4308    3020.1478    3042.6089
  3055.0410     3055.3725    3082.4164
```

S.3.6 $(\text{TS}_\delta)^\ddagger$

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==========================
        Structure    1
==========================


  1277.4015i      35.9350      60.6265      95.9263     136.3587     159.5515
   174.8011      209.5077     236.2388     269.7712     331.7841     364.7038
   507.2124      560.2996     572.7509     642.5433     731.8940     827.8466
   848.1089      904.9976     922.0008    1001.4197    1030.2790    1046.0796
  1084.5629     1099.7104    1148.3311    1157.7303    1167.7863    1175.6796
  1189.4712     1208.1048    1243.7820    1282.2635    1289.3549    1369.0337
  1380.8518     1414.0066    1416.7818    1431.4703    1440.1949    1441.5685
  1444.0957     1457.7047    1674.1527    1798.8226    2942.5555    2974.2052
  2979.7253     2981.8454    2987.8289    3017.7702    3020.2402    3030.1227
  3071.1959     3103.9219    3104.2934



==========================
        Structure    2
==========================


  1273.9513i      35.0765      74.0970      87.5065     130.7109     141.6681
   168.2041      200.7630     217.9829     288.8506     334.9681     355.9880
   507.3219      552.2573     572.5550     643.1476     729.4501     831.9487
   845.5826      905.3017     926.0439    1000.2077    1037.1985    1049.4804
  1058.9782     1109.0885    1148.4569    1156.4491    1158.3614    1175.5655
  1188.0096     1225.8792    1253.7452    1272.9967    1293.2826    1354.0206
  1377.0558     1413.4907    1422.3633    1435.0513    1440.7893    1444.2901
  1450.5438     1457.6999    1698.1510    1799.8668    2956.9958    2972.5485
  2979.7628     2988.1504    3009.8176    3013.8557    3022.6706    3033.6127
  3071.6926     3099.7681    3104.6421



==========================
```

Structure   3

========================

```
1281.8069i      45.9665      54.8653     120.0030     138.6978     166.3377
 182.2186      247.8041     265.3312     318.7944     331.2294     392.2030
 472.5942      568.8162     578.7098     651.9141     756.2012     820.0669
 848.3301      907.9030     939.0689     961.3822    1027.9326    1038.5491
1069.2207     1114.0651    1148.2500    1159.5252    1174.7443    1176.9167
1180.2361     1202.3489    1245.8120    1269.2661    1332.3987    1359.4096
1382.1592     1414.2205    1419.0204    1432.3979    1440.8945    1441.7560
1444.0726     1457.2204    1654.0805    1796.6537    2942.8174    2968.6136
2983.1686     2987.3161    3004.7617    3012.2998    3023.3718    3037.0331
3070.6365     3096.3118    3103.5451
```

Structure   4

========================

```
1265.8545i      29.7117      60.0338      96.2831     118.7970     132.9824
 140.7066      178.2947     214.8975     285.0425     311.4010     357.2808
 480.8241      551.3683     570.7602     690.3347     709.3747     783.1004
 896.7841      909.9975     918.1909    1016.3052    1032.7855    1054.6903
1081.5656     1095.0386    1148.4004    1154.0765    1156.0482    1174.4153
1200.2812     1202.1194    1260.4452    1273.0771    1286.4899    1333.7996
1386.2378     1415.9858    1424.0218    1439.6805    1443.4219    1443.9296
1455.3033     1458.0883    1704.7736    1802.1709    2952.5475    2972.5377
2983.3094     2987.5960    2992.9782    3010.9833    3015.9663    3034.7400
3070.8865     3101.7624    3103.8156
```

Structure   5

========================

```
1298.1839i      33.9904      61.2593      92.2786     136.8865     153.0895
 170.7414      205.6221     239.6387     279.0881     317.7449     363.7680
 507.1947      562.8865     572.2392     642.0331     736.1212     829.3745
 840.7156      904.7315     915.9528    1002.1730    1032.5429    1055.0620
1069.6688     1109.1619    1147.2484    1148.9930    1168.7946    1172.7393
1177.2179     1226.4202    1240.2779    1271.3776    1294.8055    1370.0782
1380.1727     1413.8193    1417.0745    1432.7789    1440.2741    1442.1010
1444.1382     1457.8087    1674.9081    1801.4360    2913.9146    2968.8403
2978.5565     2987.7794    3002.6327    3014.2049    3019.1885    3030.5189
3071.1378     3100.7318    3104.0317
```

Structure   6

========================

1294.2221i	26.2679	62.3323	98.6435	104.6520	135.2155
153.2390	178.9537	239.3589	284.5190	309.1323	353.2279
475.6476	560.9528	571.4664	690.0534	709.3823	797.5024
880.7447	909.6355	911.9510	1017.5463	1040.7247	1063.2492
1074.1417	1108.1169	1142.8139	1148.6052	1167.3265	1174.6079
1178.5405	1208.2431	1250.1593	1272.6242	1284.7175	1349.7539
1392.4402	1416.6032	1417.8287	1433.8866	1439.8299	1443.8534
1453.3098	1458.1856	1671.7242	1802.8615	2920.5426	2970.3725
2972.8266	2982.0691	2987.4460	3009.5631	3017.8881	3032.6679
3070.6895	3103.5237	3104.0993			

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==========================
        Structure    7
==========================
```

1257.5833i	52.7741	95.3557	120.0062	143.7200	171.4748
208.8391	223.0272	291.2707	302.9217	338.0577	390.6424
465.5897	563.7437	595.1259	654.5393	786.0476	804.8597
850.3895	914.4849	924.0401	966.8790	1029.0620	1046.6273
1077.9197	1106.6832	1147.8306	1159.5075	1164.1290	1177.2182
1194.1038	1223.9199	1237.8628	1260.3663	1336.9057	1354.8371
1382.5261	1408.2801	1415.3341	1429.0351	1439.8479	1441.5027
1444.0782	1456.3637	1659.9455	1797.4804	2931.6852	2968.0020
2974.3321	2983.0927	2986.6664	3021.8675	3022.6503	3029.5784
3070.2640	3103.3011	3113.8571			

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==========================
        Structure    8
==========================
```

1284.5466i	26.0456	61.0103	101.4668	128.9527	136.5725
173.7360	203.9880	259.1995	304.7797	321.2426	407.0545
429.0723	572.2619	573.4486	686.9366	749.6293	796.7482
874.9972	909.2755	926.9567	959.6863	1029.4335	1061.0684
1090.0548	1093.2042	1148.4233	1164.2147	1166.2277	1174.6421
1189.8595	1210.6420	1232.2508	1278.2063	1316.7158	1343.0115
1390.7295	1413.7458	1416.7606	1430.0784	1439.7047	1443.8369
1449.8607	1458.0775	1668.9467	1799.7604	2937.9768	2969.1439
2977.1918	2985.5761	2987.1468	3012.2138	3016.4351	3035.7010
3069.9551	3098.1624	3103.1584			

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==========================
        Structure    9
==========================
```

1284.4921i	31.3954	45.0439	90.7715	135.8519	155.7609
173.7420	230.7989	254.0215	297.2580	344.8246	399.3330
474.1763	550.8155	572.5168	647.8712	746.5200	817.0547

849.5016	902.6173	937.9456	965.5803	1028.3751	1038.4102
1080.3055	1103.7715	1148.2233	1152.4106	1165.6741	1173.0933
1177.1072	1193.1569	1242.2645	1278.0308	1333.4855	1352.4072
1380.5047	1411.2591	1429.3781	1433.6500	1440.6483	1441.0133
1444.1950	1457.6899	1665.4133	1798.2504	2948.7661	2975.4569
2983.6490	2987.8868	3000.6558	3020.5306	3027.1009	3038.6400
3071.2523	3102.4929	3104.3227			

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==========================
      Structure   10
==========================
```

1291.1732i	33.0436	54.3240	90.3930	130.1553	146.2078
176.5306	202.4061	256.7326	279.7205	340.8818	409.2477
474.4304	555.7354	575.2930	647.7384	743.7387	826.8214
845.1115	906.0319	933.9964	957.4260	1029.3961	1057.1913
1063.1267	1105.4567	1147.9132	1149.7979	1163.5071	1170.2960
1176.7355	1224.1972	1247.0310	1274.3099	1315.7717	1346.4378
1378.8375	1416.5757	1425.1634	1433.8556	1440.9251	1444.0161
1451.6833	1457.6595	1677.1032	1799.2996	2970.7377	2973.6927
2982.3764	2988.0147	3010.7773	3019.5804	3026.5861	3035.4789
3071.5176	3096.2372	3104.4932			

```
==========================
      Structure   11
==========================
```

1282.5352i	26.7013	56.7818	97.3110	104.3066	135.1107
165.5317	172.2590	244.9712	273.5654	303.7982	424.2973
447.4406	554.9763	573.0169	687.9501	739.6080	780.1301
887.8352	907.5471	922.0773	963.1567	1035.4365	1064.9035
1075.3029	1105.8816	1147.9841	1149.1441	1159.2029	1175.1467
1183.3548	1211.4667	1260.0216	1270.7683	1317.7547	1319.1219
1386.4976	1416.9164	1425.8691	1439.2502	1443.3953	1443.8609
1450.2721	1458.0754	1683.6215	1801.8153	2960.2298	2971.7881
2980.9236	2987.5264	3006.9785	3012.1098	3014.4186	3033.7688
3070.7875	3099.6006	3103.7525			

```
==========================
      Structure   12
==========================
```

1289.6588i	35.4278	63.3909	74.2543	137.8464	154.4783
181.0984	206.8719	236.6108	282.3552	330.0321	385.0751
499.9994	557.6133	593.9691	648.6091	737.6439	828.4618
846.1841	880.9191	923.4683	987.4389	1034.8545	1055.8079
1081.7557	1104.4980	1148.6655	1156.0308	1167.8549	1178.0816
1188.3976	1205.4854	1268.7068	1276.9672	1305.1131	1340.6303

```
1373.6111    1416.4982    1421.8667    1430.3426    1437.0826    1443.3525
1446.8951    1457.6907    1670.3801    1802.2045    2925.5620    2975.6763
2980.5700    2983.4845    2987.5286    3017.5237    3025.9612    3048.8697
3070.9458    3103.2567    3104.1067
```

```
==========================
         Structure  13
==========================
```

```
1294.9720i     25.4745      55.1616      69.9620     120.6151     135.6243
 170.3042     194.9101     237.9148     302.7506     312.3705     416.0923
 438.6254     553.4712     572.1460     686.4767     738.3823     793.3608
 871.2156     905.5603     924.3866     970.2046    1038.9792    1062.5253
1080.2950    1106.4989    1141.3090    1148.6876    1168.3731    1170.2233
1175.3591    1211.5112    1239.7509    1279.3004    1317.6775    1339.5843
1388.7945    1416.6658    1424.2252    1434.9705    1439.6395    1443.8290
1449.7574    1458.0942    1669.4302    1802.8166    2918.4295    2969.4523
2983.4425    2987.4484    2998.6588    3016.6071    3023.9796    3038.9147
3070.7441    3103.5233    3104.2081
```

```
==========================
         Structure  14
==========================
```

```
1290.7445i     33.1528      58.8769      74.7731     137.0041     152.0634
 177.7787     205.6206     243.3307     289.7341     316.1057     384.5785
 499.0294     557.6262     594.8452     651.2493     741.1014     829.8072
 842.7889     879.6082     919.7339     990.0252    1040.3712    1053.0880
1086.3275    1102.5495    1146.8647    1148.9585    1168.3935    1171.6785
1178.5223    1222.6382    1262.3105    1276.8278    1309.4008    1340.5006
1373.7742    1416.9725    1422.3886    1430.5800    1437.1076    1443.6193
1446.5905    1457.5441    1675.0534    1801.5625    2924.9352    2970.0429
2981.4900    2983.7388    2987.4944    3016.4355    3026.4128    3048.9930
3070.6739    3102.9328    3104.0892
```

```
==========================
         Structure  15
==========================
```

```
1270.0751i     30.9238      80.2792     106.2868     132.8845     138.9131
 167.5861     215.4999     253.0048     295.0606     324.0750     395.6401
 478.7910     563.9064     574.2599     668.0993     759.2847     812.2406
 866.1404     914.1987     920.3099     965.4794    1023.2838    1040.8122
1076.8821    1105.7631    1148.3828    1157.0145    1157.8133    1174.7978
1195.1428    1204.9178    1248.5379    1268.8507    1321.7760    1340.5875
1376.1134    1417.7461    1424.9383    1437.4099    1440.4764    1443.8310
1447.0361    1457.4176    1690.9002    1797.4194    2957.4081    2973.0837
2980.5468    2987.9726    3003.3114    3014.7194    3026.1252    3035.2129
```

```
3071.5760      3103.3581      3104.6614


              ==========================
                 Structure   16
              ==========================

1279.0032i      35.6188        66.1501        83.6840       127.5827       137.5762
 173.4234      199.3180       221.3888       296.0101       335.3624       374.7872
 499.5347      551.1521       592.0041       647.4918       732.9148       835.9900
 846.8467      873.1218       926.9459       994.0200      1036.8624      1048.8241
1070.5825     1109.8130      1148.7218      1156.1888      1158.7066      1177.9241
1186.5306     1231.0949      1263.1477      1286.8452      1298.6582      1340.0530
1356.8090     1419.6459      1424.2132      1433.7930      1442.5067      1443.4255
1448.6231     1457.6112      1697.2675      1802.7443      2957.2135      2974.1848
2982.6500     2987.8724      3000.0038      3014.2266      3028.0084      3049.0995
3071.5815     3099.8817      3103.6363


              ==========================
                 Structure   17
              ==========================

1295.1251i      24.1805        64.1036        90.1466       106.3293       138.6225
 154.3037      189.6146       247.7211       281.8392       308.0263       376.0043
 440.5703      556.6621       633.4409       702.4677       721.1774       794.6288
 868.2238      890.2589       915.0381      1024.1000      1043.1646      1058.6369
1075.2599     1108.8861      1143.2837      1148.6728      1168.2426      1177.1177
1179.5659     1232.3806      1245.1417      1285.5105      1304.3986      1329.8780
1374.1058     1417.3642      1426.8003      1435.0379      1437.7764      1443.4736
1456.2555     1457.6258      1671.1104      1803.3672      2922.0840      2968.0629
2976.9085     2979.4967      2987.7286      3017.5527      3022.9393      3053.1895
3071.2970     3103.3185      3104.2575


              ==========================
                 Structure   18
              ==========================

1293.6238i      21.5811        64.5016        88.2352       106.2289       138.9539
 157.4849      184.3333       250.5615       282.1542       305.6786       379.4171
 434.5434      556.8492       636.7911       705.6712       724.9139       791.2860
 870.3442      890.3043       917.0368      1016.7440      1042.9303      1059.1824
1085.2806     1101.2826      1144.0318      1148.6846      1167.7441      1177.8369
1178.4772     1225.7733      1255.2984      1281.3237      1304.4645      1330.4816
1373.7603     1417.5184      1427.5003      1434.9664      1438.2199      1443.6293
1456.3651     1457.6408      1673.2414      1802.6014      2925.0149      2963.3820
2976.9873     2980.6496      2987.5909      3017.6657      3024.5628      3053.7455
3070.9043     3103.7347      3104.0182


              ==========================
```

Structure   19

==========================

1274.0875i	23.1651	62.6682	87.6598	115.8029	138.0262
139.9738	176.2739	228.3455	287.4782	316.9088	372.7215
437.3168	552.3608	636.2047	708.2113	725.1844	780.6483
867.3312	912.2515	918.7818	1016.4513	1040.8993	1054.4119
1061.5989	1106.7043	1148.6373	1154.7535	1156.7371	1177.9857
1200.6171	1218.2280	1264.6992	1288.5267	1297.0382	1323.7388
1359.2911	1424.1145	1427.9562	1438.0056	1443.5497	1444.7833
1457.6919	1458.1134	1698.4139	1803.1965	2955.4447	2968.7767
2981.0030	2987.6969	2997.7174	3015.5591	3025.7351	3056.4231
3071.1698	3101.4373	3103.5326			

==========================
Structure   20
==========================

1273.9198i	22.9549	58.4146	72.3515	123.9333	140.1580
180.9929	215.6603	274.3933	298.4025	351.1701	415.5333
472.3892	554.9787	604.4343	691.6500	750.5717	820.5992
845.2123	891.4591	937.6983	959.3349	1017.7451	1061.6529
1086.5211	1095.7979	1146.8572	1148.4318	1160.5569	1168.1804
1178.0941	1193.0004	1262.3305	1286.1497	1320.0395	1344.1831
1355.2252	1419.8872	1433.5452	1437.3361	1440.7073	1443.7976
1450.3357	1457.7036	1682.5995	1799.6369	2918.1845	2979.6990
2987.1927	2997.1619	3002.4016	3025.7529	3030.9311	3064.9955
3070.3092	3103.6131	3109.9346			

==========================
Structure   21
==========================

1283.3791i	20.4465	49.3393	105.7217	121.6354	139.2961
168.8674	196.8703	257.6677	293.0579	340.6762	415.2897
469.3052	564.2668	604.8472	689.0197	746.6774	834.9595
840.4823	887.8052	936.8085	953.9527	1030.0514	1053.2345
1080.7434	1099.7966	1144.1786	1148.3730	1159.7919	1164.1260
1178.7781	1222.8817	1262.0446	1285.8499	1311.8163	1338.4983
1351.4169	1423.2906	1430.2222	1434.5813	1443.4789	1445.5570
1450.1316	1457.6402	1689.3940	1800.0217	2959.9648	2973.3778
2987.4862	2996.3902	3005.6883	3013.5383	3025.2995	3063.6139
3070.8864	3102.8260	3103.9401			

==========================
Structure   22
==========================

```
1293.1809i     23.3373     55.0247    107.6231    110.9472    141.2427
 186.1022     217.9799    257.0159    294.2052    318.6267    399.2523
 434.6864     571.7779    627.3458    721.3774    742.8340    791.4539
 868.9381     886.4806    936.0926    955.8526   1038.8751   1056.1980
1081.4086    1102.9743   1148.6171   1163.4480   1166.0618   1178.1497
1191.9013    1212.8094   1261.9890   1277.5562   1317.3705   1340.6836
1365.7145    1414.7528   1426.4999   1431.2106   1437.8696   1443.5333
1453.4559    1457.8643   1667.8174   1803.1520   2938.3427   2969.6306
2979.2339    2987.2101   2990.3536   3012.9884   3019.6142   3056.9669
3070.5122    3099.3054   3102.5456
```

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==========================
        Structure   23
==========================
```

```
1290.4561i     21.7302     54.5574     97.7625    123.1126    140.2621
 183.0789     227.1680    253.2538    294.1749    319.6075    409.5040
 421.3178     571.7250    629.0108    713.7849    758.1366    799.3662
 872.4536     885.1807    926.5656    958.7086   1038.9984   1051.3836
1081.0367    1105.5784   1148.7175   1161.6341   1164.8047   1178.0259
1190.2226    1212.6788   1254.3627   1286.1456   1317.9642   1339.7871
1365.9334    1415.0113   1427.2540   1430.9836   1438.5068   1443.4690
1454.2681    1457.9725   1669.4342   1803.1051   2938.1812   2961.4706
2979.1963    2985.5354   2987.1282   3014.2224   3024.5932   3069.2777
3070.2584    3100.4464   3102.6407
```

```
==========================
        Structure   24
==========================
```

```
1282.6722i     51.6977     62.7420     97.0360    132.8846    141.8830
 171.5824     210.7931    258.2361    301.6754    321.0682    407.0999
 480.4484     573.2533    588.6055    666.3257    763.9065    811.1704
 855.7796     892.3766    922.8217    974.5178   1007.8978   1055.1356
1082.3744    1107.7578   1147.7047   1159.9642   1162.0441   1178.2620
1199.2621    1206.4749   1265.8573   1285.6562   1320.7890   1342.7017
1352.1106    1420.4820   1427.5442   1434.3982   1442.8338   1443.4881
1446.4408    1456.8302   1675.1094   1798.3577   2958.8436   2973.1945
2981.4198    2985.8599   3003.8543   3016.9202   3026.0033   3048.0622
3069.0682    3102.8339   3104.8162
```

```
==========================
        Structure   25
==========================
```

```
1284.7926i     24.0246     52.2893     94.4018    108.5911    137.6277
 146.0357     212.3897    246.3409    272.1542    294.9722    410.8471
 456.9845     556.6625    623.9460    719.9565    732.5941    776.7429
```

866.2467	897.4873	929.4255	964.1287	1042.9253	1063.3499
1071.5708	1108.8977	1148.2420	1148.6344	1158.9821	1178.1566
1183.3683	1234.7072	1261.3390	1280.9287	1318.1858	1321.1257
1358.3481	1424.6374	1428.9490	1437.8229	1443.5505	1444.3703
1452.4376	1457.7696	1682.6800	1802.8874	2961.2179	2969.9727
2982.4285	2987.8036	3006.1642	3014.7993	3023.1728	3052.4543
3071.2705	3101.1083	3103.4728			

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==========================
        Structure  26
==========================
```

1267.3944i	33.6840	62.0707	86.9350	132.3474	169.4630
191.7781	229.0545	253.3829	307.3262	326.1557	403.6170
478.2968	558.7967	589.9191	669.6151	768.0011	804.3369
849.0431	887.8714	920.0678	970.7616	1023.4760	1068.5638
1077.9131	1095.0333	1147.6774	1149.1654	1153.5633	1169.7970
1178.9988	1216.4430	1255.7830	1286.2683	1339.0727	1345.7870
1354.2467	1418.2063	1428.6586	1435.3045	1441.0541	1443.5484
1446.4618	1454.2223	1693.3945	1796.2555	2920.7393	2975.5265
2982.5283	2985.6482	2996.8597	3025.1955	3028.7531	3047.1896
3068.8388	3104.9051	3106.2931			

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==========================
        Structure  27
==========================
```

1281.7348i	22.5514	50.8687	95.1551	101.1198	138.8103
148.2690	216.1315	241.7116	272.7375	296.5471	420.0373
444.2947	555.8738	624.6735	705.7564	750.8886	782.8510
868.7751	896.6326	923.4847	960.6169	1038.9887	1071.2418
1078.2536	1100.9027	1148.1980	1148.9248	1158.1880	1177.6486
1182.6275	1233.1080	1260.7147	1285.2697	1314.7774	1325.2848
1358.5302	1424.9481	1429.5295	1438.3036	1443.4181	1443.6351
1453.0732	1457.7396	1687.6264	1803.0648	2960.6610	2965.3307
2977.9163	2987.6800	3007.3638	3015.9564	3024.4173	3062.1182
3071.1759	3102.4518	3103.4698			

```
==========================
        Structure  28
==========================
```

1313.6085i	30.2133	59.5139	96.0729	139.3370	163.8383
181.1629	232.6623	269.8358	307.8485	340.4409	398.9452
493.3917	568.7852	581.8986	632.2543	761.2217	819.5734
848.7472	879.2994	931.9042	964.2258	1022.6380	1046.3455
1081.0120	1113.9182	1148.9560	1159.9189	1175.9571	1178.7873
1179.1737	1204.2162	1265.3554	1280.6839	1328.4444	1351.3945

1360.9197	1414.3654	1420.2121	1433.3698	1435.6186	1443.0113
1444.4781	1457.8174	1651.6484	1802.3628	2940.7845	2966.6400
2980.2759	2987.5359	2989.0050	3011.7161	3026.5721	3050.7332
3071.3550	3097.0638	3102.4690			

==========================
Structure   29
==========================

1296.1812i	19.4844	46.8108	72.2685	112.2531	139.8283
176.2781	214.0467	237.2456	290.2282	310.7518	409.0791
439.8734	553.2475	624.7652	718.1120	733.4368	783.4330
868.8888	880.9829	932.3445	967.2801	1040.5754	1070.7103
1087.8474	1093.4889	1142.2590	1148.6580	1168.0064	1169.8655
1178.3384	1223.1037	1267.9073	1274.9080	1318.0258	1340.7193
1362.1023	1422.6045	1428.6379	1434.9480	1438.0290	1443.6602
1452.1728	1457.6085	1670.5845	1802.0155	2924.0911	2972.4026
2986.1129	2987.5474	2995.9982	3023.9164	3025.7424	3053.5065
3070.8898	3103.6331	3105.8065			

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Structure   30
==========================

1297.1351i	22.6316	48.1816	78.4077	110.7861	140.6285
176.3790	213.4957	236.4693	292.6869	314.0388	420.4706
425.6962	553.8965	621.0256	700.6225	745.6264	794.6402
868.7678	880.4823	924.3473	971.4323	1040.7752	1071.2720
1080.7626	1102.1756	1140.3289	1148.7141	1168.9316	1169.4083
1178.8648	1227.4305	1251.5864	1292.0171	1314.5301	1341.5947
1363.9514	1423.0821	1427.4226	1434.5359	1437.8987	1443.5441
1452.6325	1457.6733	1667.6735	1803.1039	2921.5391	2967.6813
2977.3937	2987.7052	2995.2014	3024.8121	3030.8103	3064.3112
3071.2906	3103.3103	3107.6405			

==========================
Structure   31
==========================

1299.8249i	16.9693	66.4115	103.2227	137.6446	162.6248
187.0470	229.7070	249.9173	310.2139	324.6049	390.9620
476.5372	553.7971	570.7656	673.9567	763.3053	806.5251
856.4736	910.2782	918.0577	970.5359	1033.4501	1052.5431
1082.4621	1085.7538	1144.5531	1148.7171	1152.6672	1168.8540
1177.0606	1213.3979	1233.9687	1267.3123	1340.1458	1342.9111
1376.1148	1416.7940	1426.4806	1436.6615	1439.7475	1443.3277
1443.8598	1457.7009	1695.4503	1803.1271	2916.7249	2973.5359
2980.7206	2987.6963	2994.3796	3019.5623	3026.9414	3033.9597

```
3071.2967      3100.0837      3103.9145


                    ==========================
                          Structure   32
                    ==========================


1280.8749i       54.1154        56.9197       107.8850       143.0737       186.2681
 196.1019       215.5043       295.5571       301.9566       327.3899       391.6196
 494.1183       561.6727       588.1999       626.7062       784.0673       800.3738
 854.2035       871.5303       918.4278       975.6164      1024.9216      1054.1020
1088.2342      1105.3959      1148.6934      1163.0764      1169.2444      1179.3875
1195.2495      1234.8811      1246.3584      1283.3660      1339.6274      1345.3151
1365.8376      1405.4984      1413.3907      1429.1388      1435.4214      1442.4994
1445.9083      1456.7821      1659.1697      1798.2459      2930.7682      2970.2695
2974.7044      2983.2938      2986.7216      3021.7276      3022.4946      3031.3603
3071.4264      3101.2374      3109.4169


                    ==========================
                          Structure   33
                    ==========================


1260.2385i       64.2033        68.6875       123.2873       154.6461       209.1511
 211.8320       253.9134       263.1481       330.6113       339.0618       418.7767
 524.0206       538.4821       574.0727       594.5955       738.7744       802.5910
 823.7547       889.4749       937.9837       966.6609      1029.9151      1065.2632
1085.6838      1113.1780      1140.1399      1150.0283      1161.6474      1177.2117
1180.1994      1205.5055      1244.2753      1269.9877      1330.9162      1359.5805
1380.4571      1413.6392      1415.4586      1431.6483      1439.7240      1446.2802
1458.9175      1464.8148      1661.6931      1815.8784      2943.2433      2963.7212
2965.6446      2974.6307      3005.8674      3015.7600      3024.6659      3038.8861
3044.2739      3088.2528      3096.7282


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                          Structure   34
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1275.6573i       47.5262        60.1331       101.4501       124.8876       165.1730
 195.3940       229.9027       245.4120       258.4997       326.7643       414.6739
 529.4324       540.4340       563.1601       587.6807       712.7909       795.8541
 833.5630       888.0603       923.6506      1010.2610      1040.6262      1076.8603
1085.3344      1103.4766      1139.5714      1145.6079      1161.4305      1168.7883
1191.1989      1212.3773      1240.6441      1282.4317      1291.2624      1369.1961
1378.0950      1407.6111      1416.9796      1431.1070      1440.1361      1447.9605
1458.3002      1463.5353      1674.2399      1820.4288      2942.1755      2962.7941
2968.5461      2977.0511      2983.1017      3008.0543      3018.8865      3031.5827
3045.5514      3089.6998      3105.1203


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                   Structure   35
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1235.4298i      70.3040     121.5069     136.7658     153.2496     215.5197
 224.6222      236.9811     294.1476     304.6887     361.3348     424.1222
 523.8655      530.4729     582.3400     598.9355     763.0225     795.9600
 829.3955      893.9202     928.1629     972.0538    1038.3109    1075.5930
1087.4650     1106.2564    1140.1246    1151.7195    1156.8477    1165.3674
1188.5933     1224.4273    1242.9318    1256.4314    1335.6631    1352.5500
1380.4307     1407.9789    1415.1605    1428.7552    1441.5902    1445.5934
1458.8218     1464.8040    1668.1795    1815.8973    2933.0437    2962.7426
2965.1684     2967.8639    2986.5782    3018.3479    3025.3440    3037.6811
3043.9227     3088.5454    3117.7331


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                   Structure   36
            =========================

1268.2998i      32.0816      77.1540      93.9437     117.3155     139.2187
 196.1081      217.7169     265.4159     305.4350     328.1348     420.5294
 503.7008      538.5348     572.9988     593.8380     746.0760     797.5449
 847.7489      887.7927     926.2493     964.6462    1048.6500    1083.6226
1092.7509     1096.3100    1138.4646    1146.3588    1164.9641    1166.3779
1191.2446     1213.1568    1231.8053    1284.2006    1312.2545    1342.4717
1388.6335     1409.1994    1416.1092    1429.3647    1446.2374    1448.8226
1457.9081     1462.4227    1672.3355    1821.6527    2938.7963    2963.3689
2969.2672     2972.2223    2990.3314    3007.1342    3012.7397    3038.8561
3046.3185     3089.9141    3099.1529


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                   Structure   37
            =========================

1274.2277i      46.5283      76.6080      95.8807     121.3860     150.8987
 193.4750      208.1392     238.8257     275.0145     335.0786     406.6398
 531.0688      547.7289     552.6199     584.6431     713.5945     785.7910
 848.9401      881.4114     926.9935    1012.8653    1048.5130    1057.7227
1080.7764     1110.3440    1139.8244    1149.7560    1155.9814    1158.5575
1191.8865     1224.7585    1253.5836    1275.8505    1293.7749    1354.9341
1374.3311     1407.1477    1422.1192    1434.4533    1448.0651    1450.7584
1458.4039     1463.8417    1699.8285    1821.1322    2954.8102    2961.9630
2968.0883     2976.5076    3007.7242    3013.0465    3020.9093    3037.3620
3045.3948     3089.7133    3100.5938


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                   Structure   38
            =========================
```

1265.2358i	36.8203	71.6912	100.4624	101.5691	131.9964
146.4532	197.5021	222.4474	260.1955	341.0440	396.0481
531.5899	533.6178	551.5795	588.1564	710.4642	788.5602
842.0788	912.0094	915.7357	1029.6305	1047.0192	1071.1371
1088.5511	1096.0033	1138.6562	1146.4002	1153.3022	1156.3522
1203.2542	1203.5706	1256.4717	1277.2840	1287.1866	1331.3547
1383.0265	1410.0234	1424.2427	1441.8760	1447.0712	1453.9920
1458.1602	1461.7170	1706.0122	1823.6545	2950.2917	2958.4755
2967.7622	2988.8220	2991.1753	2999.7110	3017.4318	3038.8179
3044.5029	3089.8843	3103.4770			

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        Structure  39
==========================
```

1297.6227i	35.0228	76.2788	93.9238	107.4237	124.8862
159.3082	199.1822	233.2389	292.8122	307.6220	403.6702
522.4327	534.0635	565.1257	587.8607	710.4336	803.8191
840.2196	894.1657	912.4682	1031.7530	1065.1240	1065.9966
1084.8957	1107.8029	1138.9272	1140.6346	1149.7763	1167.2352
1178.7343	1211.5303	1251.9093	1270.4263	1286.5177	1347.5714
1389.6955	1411.4281	1417.9061	1433.5518	1446.9920	1451.3851
1458.4209	1462.3700	1671.3745	1824.6739	2918.7733	2956.8974
2967.2523	2970.4729	2987.3450	2997.9841	3018.9328	3036.5365
3043.9124	3089.3324	3105.3336			

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        Structure  40
==========================
```

1301.8698i	44.7799	61.9159	104.3343	123.4342	156.5029
194.9315	223.3195	251.6875	266.7370	315.4541	413.9173
527.7814	543.1583	560.3772	590.8864	717.2769	792.2703
835.5507	883.6104	917.7379	1011.0178	1052.9348	1063.5605
1082.1394	1112.2068	1139.4233	1143.8244	1155.2958	1169.6150
1175.0308	1227.4288	1240.9045	1271.9616	1295.9804	1370.7985
1377.2604	1407.2552	1417.1551	1432.6367	1441.8664	1447.7465
1458.2601	1463.4682	1674.2565	1822.6105	2909.8961	2960.8421
2967.3846	2971.9139	3005.4930	3010.6240	3017.0225	3033.1851
3044.5982	3089.1778	3101.2266			

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        Structure  41
==========================
```

1284.8670i	34.6686	47.8362	96.6029	122.1775	180.7533
198.3249	240.5989	250.7111	290.9043	356.2231	421.1913
524.2128	533.3488	548.4715	582.7509	728.8067	798.2801

823.1629	887.2743	935.7474	973.7892	1029.1048	1076.2873
1084.2208	1108.6443	1139.1369	1142.2729	1160.9403	1167.6496
1176.6381	1196.8435	1239.0518	1280.9422	1332.7575	1353.9641
1378.1446	1406.1687	1427.8781	1433.3768	1439.8468	1447.8649
1458.5286	1463.5528	1665.0692	1819.9144	2956.4976	2965.6146
2969.8075	2979.4316	3004.3280	3013.9229	3021.6142	3037.9193
3045.0732	3089.5589	3100.3529			

==========================
Structure   42
==========================

1288.0128i	32.7136	72.4967	94.1361	104.0594	117.6257
174.7019	198.0949	250.3542	269.1534	316.4937	451.0862
504.4783	534.0781	558.0346	591.4827	734.3001	783.7312
848.8670	895.9542	922.2455	967.9623	1059.3985	1074.0213
1087.8864	1105.8944	1138.9080	1144.6639	1151.3623	1159.5331
1184.0978	1213.8429	1258.1502	1277.2877	1314.2874	1318.3710
1383.2926	1411.2598	1425.3941	1442.4939	1446.2922	1448.9656
1458.2766	1462.0266	1679.8411	1823.4838	2958.6741	2959.9723
2967.4916	2986.2378	3001.5539	3008.0827	3013.1056	3037.5977
3044.0321	3089.7167	3098.1930			

==========================
Structure   43
==========================

1300.1062i	45.4192	54.2132	91.6137	120.0222	169.7861
197.2067	213.3028	255.5419	276.8001	351.2279	431.9662
523.9355	534.9647	557.4231	582.2326	729.8546	789.5410
838.8664	886.0101	933.2469	959.3911	1053.8843	1060.6047
1081.6206	1110.0724	1139.4765	1146.1415	1154.0722	1165.2093
1174.2506	1223.0252	1247.1208	1277.2243	1314.8510	1348.0457
1376.4004	1408.9998	1424.4583	1432.8830	1447.7836	1452.1755
1458.2571	1463.3899	1670.5181	1820.9416	2964.0580	2968.0034
2973.5355	2977.9448	3008.1091	3012.9893	3028.7302	3036.3715
3044.7069	3089.5111	3093.4555			

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Structure   44
==========================

1301.7045i	28.9302	66.6907	75.5471	112.8179	124.7148
190.4401	206.6100	245.0558	294.2938	323.5601	438.7598
502.9382	534.6734	552.7797	590.7900	732.2545	797.1291
843.7001	881.0448	923.2897	978.3059	1058.4406	1074.8817
1091.9124	1106.3292	1138.8145	1139.5716	1148.7148	1168.7243
1170.8371	1214.1310	1240.2085	1284.5124	1312.7012	1339.5892

```
1385.8100    1411.1676    1423.8701    1435.4237    1445.6867    1448.2951
1458.2997    1462.3999    1667.5057    1824.5423    2917.1099    2957.0281
2966.8158    2988.8408    3001.2990    3005.4363    3022.0445    3042.1339
3043.9594    3089.1286    3102.6099
```

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Structure   45
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```
1260.9198i     44.1990     92.7366    113.8047    133.9315    136.9822
 202.5117    213.5755    254.1678    298.6210    326.4997    433.6576
 527.9861    530.9072    566.6892    579.0125    749.3368    777.8053
 845.3445    898.6593    923.6988    974.6201   1030.9804   1079.1423
1084.1809   1105.8213   1139.7098   1147.7600   1158.3892   1160.6449
1203.3095   1206.7774   1243.5043   1269.9987   1323.2744   1339.9329
1375.6957   1408.3402   1424.4509   1435.9058   1446.2933   1447.9271
1458.5281   1464.1166   1698.9541   1820.6086   2953.1350   2961.6076
2967.4581   2980.5840   3001.7066   3009.4637   3020.3169   3038.7674
3045.2790   3089.2349   3109.7316
```

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Structure   46
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```
1259.7316i     49.9467     63.3141     99.8362    124.8695    173.6471
 197.0422    202.9357    285.5801    324.2159    350.3561    455.4139
 480.7262    551.6711    566.0954    711.1046    715.6598    788.7816
 819.6799    895.0865    938.2778    959.6032   1031.3299   1067.1429
1091.7730   1104.8998   1138.6354   1142.9375   1160.5136   1166.5199
1174.5400   1191.4298   1258.6073   1285.5039   1315.0064   1341.6927
1357.1177   1419.6982   1437.8169   1441.4443   1448.2893   1452.9252
1464.1299   1467.3421   1686.5567   1813.3432   2941.2888   2969.0062
2971.4405   3004.1542   3008.3654   3021.7886   3030.2863   3050.3678
3063.4056   3089.2737   3115.7767
```

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Structure   47
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```
1289.4707i     47.7109     61.5951    107.1585    115.2627    156.2913
 161.6869    203.0508    256.2754    279.5131    333.6466    394.5694
 468.6762    556.0111    585.2156    707.7657    711.2717    788.7944
 831.7337    894.5199    916.7389   1014.8924   1043.7528   1059.4913
1087.3404   1114.1681   1135.7404   1141.9080   1162.5013   1168.2791
1179.1598   1218.8747   1250.3658   1273.7529   1299.9809   1330.2733
1369.4798   1417.7788   1433.8230   1442.9372   1446.2570   1454.8092
1463.2927   1468.2755   1671.5792   1820.3055   2929.0507   2966.2729
2968.9017   2976.3589   2998.7501   3016.3206   3020.6270   3047.6400
```

```
3057.0851     3088.6738     3107.3008


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                         Structure   48
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 1282.5037i      49.9334       56.8676      101.9836      126.6716      157.7309
  192.7431      199.4748      231.5101      308.6695      329.2444      429.4737
  471.8229      553.7277      565.4144      697.4512      728.8003      781.7761
  826.6755      887.7104      926.9430      995.4297     1035.2730     1055.7241
 1077.7220     1118.6486     1140.5671     1150.5394     1160.7356     1170.2103
 1185.6617     1194.6373     1261.4865     1278.8112     1301.1524     1331.3945
 1374.8181     1418.3045     1432.6157     1442.5808     1448.0518     1449.1864
 1462.7786     1465.3803     1672.4178     1816.7135     2950.4067     2960.8218
 2969.7000     2990.0132     3003.5088     3016.1446     3018.7318     3049.4502
 3059.9601     3088.7907     3104.1632


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                         Structure   49
                    ==========================


 1287.0938i      50.6174       57.8241      104.1139      122.5041      158.5302
  194.8381      196.4488      239.2974      296.6135      332.6076      433.0808
  471.4624      557.8595      564.0907      694.6966      733.3185      779.6852
  826.7658      885.1556      923.5506      995.9484     1039.9508     1052.5437
 1095.0139     1109.4838     1135.6997     1142.2766     1162.2452     1169.7866
 1176.8589     1209.8157     1261.0265     1270.4946     1309.2887     1331.3019
 1376.4844     1418.8379     1431.9365     1442.0270     1448.3529     1449.7208
 1462.3888     1465.2908     1668.5819     1816.7566     2934.2483     2964.2211
 2970.5059     2997.5239     3005.7954     3014.8172     3021.0588     3050.9461
 3058.8840     3089.5261     3104.2507


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                         Structure   50
                    ==========================


 1268.7368i      37.8997       72.0089      104.1161      129.6170      171.4396
  193.5701      207.6496      250.0514      308.0818      339.0793      449.5202
  472.2529      552.2288      583.9605      696.9219      726.2038      791.9376
  832.1211      884.0174      932.0517      963.4831     1047.7293     1072.8034
 1084.0192     1109.0326     1133.7702     1140.6983     1161.1381     1166.6576
 1174.7505     1220.7502     1259.5115     1265.0425     1320.4584     1334.3331
 1356.2566     1421.1092     1437.0472     1443.6740     1446.9718     1454.0034
 1465.2766     1468.1778     1674.3812     1819.2555     2929.6010     2968.2134
 2971.7163     3001.4604     3008.6447     3023.6609     3025.8086     3049.2581
 3058.3260     3088.9104     3108.4127


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```

Structure   51
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      1279.2660i   48.3815   68.5556   105.7211   115.9056   133.5083
       160.2766   205.1613   220.5846   298.7753   343.9080   385.9001
       469.1010   552.4417   583.6334   708.6764   712.4558   775.2572
       831.8648   913.0866   918.0617   1011.0294   1046.2254   1054.3982
      1061.6528   1120.1436   1141.0655   1151.5720   1156.5166   1162.7165
      1197.5385   1214.4525   1256.7607   1283.8570   1293.0801   1324.7025
      1354.3711   1424.4799   1442.3506   1443.1389   1447.5949   1455.5486
      1463.5002   1468.2370   1696.9623   1820.5213   2955.5390   2965.4906
      2967.9965   2997.2404   3001.2627   3016.9945   3021.6557   3045.9828
      3059.4001   3088.2700   3103.1906

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                        Structure   52
                    =========================

      1284.8519i   52.1703   85.4196   114.7468   122.9152   168.5954
       179.1892   199.2171   259.0065   313.4858   341.5558   452.2715
       478.2096   564.7829   567.0340   709.1214   716.2268   782.3668
       833.5841   888.2638   938.0205   953.3280   1047.5155   1055.2507
      1093.8891   1100.2248   1135.5160   1141.7569   1157.9016   1158.2979
      1176.0608   1218.6753   1260.3159   1282.3950   1314.8892   1332.6840
      1353.7468   1420.6993   1436.8896   1447.0595   1448.2180   1449.6884
      1463.3159   1465.0887   1688.3660   1813.8697   2961.1326   2969.6338
      2970.7715   3002.7529   3010.5800   3012.4592   3023.2784   3049.8367
      3062.2571   3089.3344   3107.2902

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                        Structure   53
                    =========================

      1304.6696i   49.7626   58.5263   105.3428   119.2313   146.3547
       166.5598   203.6984   254.6713   282.4520   332.2565   393.6009
       469.0644   555.2973   585.2806   706.2799   713.2387   787.6070
       831.8974   894.2477   914.0836   1015.2744   1046.4901   1058.9675
      1079.2698   1118.3546   1136.5768   1141.5020   1163.3864   1168.6284
      1177.6223   1227.9563   1237.2765   1279.6477   1297.7261   1329.7047
      1369.2617   1417.8814   1434.2022   1443.0273   1446.3461   1454.8046
      1463.3782   1468.5228   1671.3820   1822.0549   2921.8764   2961.0470
      2967.5073   2983.1573   2997.9916   3017.8769   3019.8591   3045.9725
      3057.8225   3087.8013   3105.1269

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                        Structure   54
                    =========================

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```
1289.3940i      40.0940      54.6676     103.6484     131.4130     161.9117
 203.6652     211.2284     258.2880     318.7867     326.7888     414.2138
 472.9110     568.6192     585.5255     696.1252     739.0551     787.7856
 833.7555     890.3410     934.8760     951.9044    1039.7784    1065.3178
1078.2138    1117.5861    1141.0842    1151.6198    1165.8761    1171.2684
1190.4036    1208.5283    1253.7911    1270.4596    1318.4277    1339.4717
1362.1855    1414.6626    1428.6151    1442.7834    1445.8321    1452.9895
1463.2357    1467.1924    1673.0296    1820.1502    2940.3195    2957.0223
2966.6910    2984.4150    3009.3255    3011.2829    3020.5206    3044.8941
3065.7747    3087.3539    3098.0691
```

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Structure 55
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```
1286.3218i      49.5232      58.1385     117.0816     130.2483     163.2660
 202.9830     210.8999     259.4141     319.2531     331.6956     411.1425
 474.4351     568.6669     585.0179     697.8659     735.7898     797.6071
 838.9732     890.2002     926.0792     954.5409    1041.8111    1059.6960
1078.1748    1119.7336    1141.1827    1151.1291    1162.6760    1169.2850
1187.9525    1211.8989    1244.6584    1279.5952    1315.9573    1339.0684
1361.3728    1415.7998    1429.4895    1442.2158    1445.1825    1453.3503
1462.8650    1467.5690    1671.2761    1820.1760    2938.5769    2965.2411
2967.4920    2976.5838    3003.0278    3015.1879    3017.0133    3045.3161
3067.8254    3087.4167    3103.2076
```

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Structure 56
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```
1299.5036i      42.5181      81.9433     103.7765     129.6273     174.8131
 202.2830     218.8498     266.2106     303.6280     332.4348     424.4608
 521.7972     528.0698     553.5373     577.7924     754.5503     782.7287
 832.0135     891.0375     921.5520     980.8862    1049.7823    1073.9757
1086.1371    1095.1121    1137.5380    1140.0094    1148.1199    1151.2203
1172.1976    1221.2435    1233.0959    1266.2914    1339.6638    1346.8755
1376.1056    1406.3520    1425.6379    1435.3735    1440.0707    1447.4688
1458.6601    1464.1030    1693.0180    1825.0581    2911.4344    2960.5325
2967.1900    2979.7922    2991.3582    3006.7736    3027.3387    3036.7826
3044.3394    3088.5522    3111.5352
```

==========================
Structure 57
==========================

```
1286.8856i      49.6382      66.6291      95.7438     121.4088     133.0825
 186.8040     200.4043     213.4618     315.0633     340.7568     418.4575
 471.1377     551.4967     563.8158     697.0880     728.7573     771.7195
```

841.5416	878.6911	927.3755	996.1709	1034.8870	1049.5423
1079.4322	1117.8056	1140.8510	1146.1746	1156.6413	1160.9317
1181.6870	1221.9266	1258.6661	1283.2860	1300.8879	1327.4581
1360.3399	1424.8657	1438.6241	1445.4120	1448.1334	1451.8403
1463.1452	1465.2601	1697.1705	1818.4977	2960.8291	2969.1779
2973.3947	2998.8737	3009.0151	3012.2030	3029.2291	3048.6801
3059.7687	3088.6390	3097.6572			

```
==========================
      Structure   58
==========================
```

1295.6786i	38.5597	60.9137	96.7247	114.3637	152.0882
179.4390	206.1836	248.9155	268.8743	328.9235	443.5766
472.8414	557.9614	582.2054	698.0464	729.5505	775.8297
832.9654	897.5153	927.5387	958.7970	1049.5216	1068.8472
1069.1417	1117.9234	1140.3337	1142.6573	1157.5833	1163.5847
1182.7046	1229.2724	1253.7156	1275.7003	1316.7892	1321.4871
1352.2575	1424.9255	1440.3479	1445.0893	1446.2471	1452.3474
1463.3732	1467.4681	1678.0209	1820.6224	2962.2116	2965.1828
2967.2744	3002.9765	3011.1431	3012.9622	3018.5494	3045.6906
3059.2613	3088.0961	3099.4905			

```
==========================
      Structure   59
==========================
```

1285.3935i	43.8244	61.2053	97.0950	126.3815	131.6325
183.0914	206.9617	249.0083	272.3395	330.9996	441.3538
472.8297	556.3648	581.6865	698.5668	727.8040	778.0682
842.2036	895.8818	922.6055	956.2197	1046.5086	1068.6346
1077.6151	1116.3608	1139.0293	1143.1806	1156.3563	1161.5323
1184.9875	1225.5533	1253.9570	1279.7740	1311.9152	1325.6186
1351.8617	1425.6953	1441.3938	1443.9531	1446.6301	1452.7837
1463.4734	1467.6663	1687.4359	1820.5155	2958.5094	2965.2637
2967.7885	2998.2440	3004.4249	3018.0155	3019.0980	3045.6782
3062.2952	3088.0123	3104.5498			

```
==========================
      Structure   60
==========================
```

1307.6294i	33.8097	56.6201	88.9977	133.9135	150.3582
194.3693	206.0015	243.1381	305.7823	332.2069	423.8892
469.5854	553.1012	581.7880	696.1534	728.5283	788.3726
837.4903	884.3855	923.0558	962.4330	1047.0747	1072.3748
1082.7255	1108.3122	1132.0457	1141.6224	1162.5406	1167.5328
1173.0265	1225.1211	1237.7869	1285.4458	1312.1644	1341.1224

1355.9857	1423.1819	1434.4882	1442.1350	1445.9174	1452.9959
1463.3994	1468.0834	1668.3149	1822.1644	2920.0601	2966.5713
2970.2681	2995.0128	2998.0853	3020.6641	3026.5652	3045.7096
3066.1707	3087.6360	3108.7903			

===========================
Structure   61
===========================

1308.3016i	52.9072	70.1657	103.0758	126.6126	174.7461
199.8946	208.5824	316.2017	322.4826	342.2169	410.6037
478.6100	561.2063	574.7709	706.3708	731.0211	789.7916
821.9341	889.4818	930.1126	951.3287	1032.4807	1050.1069
1094.0668	1107.6516	1136.5347	1141.5613	1159.6347	1171.9692
1177.8273	1208.1805	1249.0835	1275.9996	1326.3303	1337.0534
1366.1897	1414.6470	1429.8499	1443.0331	1447.0450	1449.8219
1463.6872	1466.1098	1691.5755	1818.1590	2934.2085	2962.9250
2967.2007	2998.6916	3007.1958	3012.4168	3017.2005	3045.8011
3067.9291	3087.0269	3097.8016			

===========================
Structure   62
===========================

1261.4432i	49.8956	76.8702	109.5498	119.8854	149.7394
184.9531	201.8004	270.0620	310.4991	343.2663	410.4712
472.2041	549.4243	563.2280	697.8659	739.7668	784.4822
826.6922	898.6805	927.4386	971.2977	1041.4651	1062.4149
1079.1291	1110.3305	1135.1187	1141.5970	1163.8808	1169.4278
1177.2095	1210.4242	1242.9596	1282.9382	1322.5090	1336.5454
1360.0576	1424.0163	1434.9700	1439.1723	1448.0858	1452.0356
1461.6409	1464.9204	1678.6419	1814.9669	2941.8126	2971.4016
2974.7174	2999.4839	2999.8987	3021.3318	3029.3177	3054.9495
3059.2967	3091.3949	3113.8995			

===========================
Structure   63
===========================

1296.3479i	39.3049	64.5952	104.2047	118.3181	147.6173
186.2201	193.8875	260.6300	302.8334	336.1233	430.6670
472.3974	558.0780	564.1046	695.1944	736.1834	769.6511
835.7405	902.6442	931.5238	973.9184	1025.1261	1063.5813
1078.2884	1115.8101	1140.0351	1149.9926	1161.6963	1167.5889
1194.4102	1202.0935	1264.6031	1286.7300	1313.8110	1330.6712
1354.6621	1422.5410	1435.8959	1439.7836	1448.0934	1449.6636
1461.8490	1464.8684	1661.7899	1813.8376	2962.6282	2967.1559
2972.5141	2997.5321	3011.4790	3014.0391	3021.5381	3053.1784

```
3058.0532     3090.2276     3122.0268
```

```
              =========================
                    Structure  64
              =========================
```

```
1287.6733i       31.9957       75.6198       92.5181      135.4597      177.9738
 187.1984       216.2425      235.2771      299.4130      348.8200      439.0844
 454.2016       562.2027      564.9834      693.8243      757.6687      787.3606
 818.2885       896.1034      936.7593      965.7394     1040.7871     1069.1060
1079.3293      1115.3026     1138.5473     1145.5617     1158.6064     1167.2079
1180.8582      1190.5975     1259.4041     1270.6626     1328.5312     1338.1274
1346.3782      1425.6423     1436.5701     1443.2321     1445.4135     1453.3809
1462.4519      1464.5738     1666.9421     1818.3514     2923.0811     2967.1788
2970.2835      2991.8850     2995.7387     3019.3296     3027.5177     3050.9340
3053.4915      3089.8122     3116.3811
```

S.4. Recrossing and Semiclassical Transmission Coefficients

S.4.1 ($R_{\alpha'}$)

```
----------------------------------------
  T (K)  |    Gamma    |    Kappa    |
         |     CVT     |   CVT/SCT   |
----------------------------------------
  200.00 |  7.1064E-01 |  3.8099E+02 |
  298.15 |  7.4204E-01 |  1.2720E+01 |
  300.00 |  7.4248E-01 |  1.2304E+01 |
  500.00 |  7.7424E-01 |  2.3632E+00 |
  750.00 |  7.9031E-01 |  1.4544E+00 |
 1000.00 |  7.9605E-01 |  1.2325E+00 |
 1100.00 |  7.9705E-01 |  1.1882E+00 |
 1150.00 |  7.9738E-01 |  1.1708E+00 |
 1200.00 |  7.9763E-01 |  1.1557E+00 |
 1250.00 |  7.9781E-01 |  1.1426E+00 |
 1300.00 |  7.9793E-01 |  1.1311E+00 |
 1350.00 |  7.9799E-01 |  1.1209E+00 |
 1400.00 |  7.9801E-01 |  1.1120E+00 |
 1450.00 |  7.9800E-01 |  1.1040E+00 |
 1500.00 |  7.9796E-01 |  1.0968E+00 |
 1550.00 |  7.9789E-01 |  1.0904E+00 |
 1600.00 |  7.9780E-01 |  1.0846E+00 |
 1650.00 |  7.9769E-01 |  1.0793E+00 |
 1700.00 |  7.9756E-01 |  1.0745E+00 |
 1800.00 |  7.9728E-01 |  1.0662E+00 |
 1900.00 |  7.9696E-01 |  1.0592E+00 |
 2000.00 |  7.9663E-01 |  1.0532E+00 |
 2500.00 |  7.9483E-01 |  1.0338E+00 |
----------------------------------------
```

S.4.2 (R_{α})

```
----------------------------------------
  T (K)  |    Gamma    |    Kappa    |
         |     CVT     |   CVT/SCT   |
----------------------------------------
  200.00 |  9.9930E-01 |  7.7712E+01 |
  298.15 |  9.9945E-01 |  7.4009E+00 |
  300.00 |  9.9946E-01 |  7.2276E+00 |
  500.00 |  9.9959E-01 |  2.0953E+00 |
  750.00 |  9.9967E-01 |  1.3987E+00 |
 1000.00 |  9.9971E-01 |  1.2097E+00 |
 1100.00 |  9.9972E-01 |  1.1707E+00 |
 1150.00 |  9.9972E-01 |  1.1553E+00 |
 1200.00 |  9.9972E-01 |  1.1419E+00 |
```

```
1250.00 |  9.9973E-01 | 1.1302E+00 |
1300.00 |  9.9973E-01 | 1.1198E+00 |
1350.00 |  9.9973E-01 | 1.1107E+00 |
1400.00 |  9.9973E-01 | 1.1026E+00 |
1450.00 |  9.9974E-01 | 1.0954E+00 |
1500.00 |  9.9974E-01 | 1.0889E+00 |
1550.00 |  9.9974E-01 | 1.0831E+00 |
1600.00 |  9.9974E-01 | 1.0778E+00 |
1650.00 |  9.9974E-01 | 1.0730E+00 |
1700.00 |  9.9974E-01 | 1.0686E+00 |
1800.00 |  9.9975E-01 | 1.0610E+00 |
1900.00 |  9.9975E-01 | 1.0546E+00 |
2000.00 |  9.9975E-01 | 1.0492E+00 |
2500.00 |  9.9975E-01 | 1.0313E+00 |
----------------------------------------
```

S.4.3 ($\mathbf{R}_\beta$)

```
----------------------------------------
  T (K)   |   Gamma   |   Kappa   |
          |   CVT     |  CVT/SCT  |
----------------------------------------
  200.00 |  9.7491E-01 | 7.4258E+01 |
  298.15 |  9.8883E-01 | 6.6740E+00 |
  300.00 |  9.8898E-01 | 6.5155E+00 |
  500.00 |  9.9685E-01 | 1.9195E+00 |
  750.00 |  9.9898E-01 | 1.3219E+00 |
 1000.00 |  9.9954E-01 | 1.1634E+00 |
 1100.00 |  9.9964E-01 | 1.1311E+00 |
 1150.00 |  9.9968E-01 | 1.1185E+00 |
 1200.00 |  9.9971E-01 | 1.1074E+00 |
 1250.00 |  9.9974E-01 | 1.0978E+00 |
 1300.00 |  9.9977E-01 | 1.0894E+00 |
 1350.00 |  9.9979E-01 | 1.0820E+00 |
 1400.00 |  9.9980E-01 | 1.0755E+00 |
 1450.00 |  9.9982E-01 | 1.0696E+00 |
 1500.00 |  9.9983E-01 | 1.0645E+00 |
 1550.00 |  9.9984E-01 | 1.0598E+00 |
 1600.00 |  9.9985E-01 | 1.0555E+00 |
 1650.00 |  9.9986E-01 | 1.0518E+00 |
 1700.00 |  9.9987E-01 | 1.0483E+00 |
 1800.00 |  9.9988E-01 | 1.0422E+00 |
 1900.00 |  9.9990E-01 | 1.0373E+00 |
 2000.00 |  9.9990E-01 | 1.0330E+00 |
 2500.00 |  9.9993E-01 | 1.0194E+00 |
----------------------------------------
```

S.4.4 $(\mathbf{R}_\gamma)$

```
----------------------------------------
  T (K)  |    Gamma    |    Kappa    |
         |     CVT     |   CVT/SCT   |
----------------------------------------
  200.00 | 5.6022E-01  | 4.7494E+01  |
  298.15 | 6.3616E-01  | 5.5974E+00  |
  300.00 | 6.3716E-01  | 5.4799E+00  |
  500.00 | 7.0199E-01  | 1.8449E+00  |
  750.00 | 7.3046E-01  | 1.3121E+00  |
 1000.00 | 7.4084E-01  | 1.1646E+00  |
 1100.00 | 7.4295E-01  | 1.1340E+00  |
 1150.00 | 7.4375E-01  | 1.1220E+00  |
 1200.00 | 7.4441E-01  | 1.1114E+00  |
 1250.00 | 7.4497E-01  | 1.1022E+00  |
 1300.00 | 7.4543E-01  | 1.0941E+00  |
 1350.00 | 7.4582E-01  | 1.0869E+00  |
 1400.00 | 7.4614E-01  | 1.0805E+00  |
 1450.00 | 7.4640E-01  | 1.0748E+00  |
 1500.00 | 7.4661E-01  | 1.0697E+00  |
 1550.00 | 7.4678E-01  | 1.0651E+00  |
 1600.00 | 7.4692E-01  | 1.0610E+00  |
 1650.00 | 7.4702E-01  | 1.0572E+00  |
 1700.00 | 7.4710E-01  | 1.0538E+00  |
 1800.00 | 7.4719E-01  | 1.0478E+00  |
 1900.00 | 7.4722E-01  | 1.0427E+00  |
 2000.00 | 7.4720E-01  | 1.0385E+00  |
 2500.00 | 7.4668E-01  | 1.0244E+00  |
----------------------------------------
```

S.4.5 $(\mathbf{R}_\delta)$

```
----------------------------------------
  T (K)  |    Gamma    |    Kappa    |
         |     CVT     |   CVT/SCT   |
----------------------------------------
  200.00 | 9.8554E-01  | 1.4591E+02  |
  298.15 | 9.9403E-01  | 7.4415E+00  |
  300.00 | 9.9412E-01  | 7.2361E+00  |
  500.00 | 9.9854E-01  | 1.8953E+00  |
  750.00 | 9.9965E-01  | 1.3046E+00  |
 1000.00 | 9.9990E-01  | 1.1528E+00  |
 1100.00 | 9.9994E-01  | 1.1222E+00  |
 1150.00 | 9.9995E-01  | 1.1102E+00  |
 1200.00 | 9.9996E-01  | 1.0998E+00  |
 1250.00 | 9.9997E-01  | 1.0907E+00  |
 1300.00 | 9.9998E-01  | 1.0828E+00  |
```

```
1350.00 |  9.9998E-01 |  1.0759E+00  |
1400.00 |  9.9999E-01 |  1.0697E+00  |
1450.00 |  9.9999E-01 |  1.0641E+00  |
1500.00 |  9.9999E-01 |  1.0593E+00  |
1550.00 |  9.9999E-01 |  1.0549E+00  |
1600.00 |  1.0000E+00 |  1.0509E+00  |
1650.00 |  1.0000E+00 |  1.0473E+00  |
1700.00 |  1.0000E+00 |  1.0441E+00  |
1800.00 |  1.0000E+00 |  1.0385E+00  |
1900.00 |  1.0000E+00 |  1.0338E+00  |
2000.00 |  1.0000E+00 |  1.0299E+00  |
2500.00 |  1.0000E+00 |  1.0171E+00  |
----------------------------------------
```

Table S.1.: All conformers of MP, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4)$	U_{jx}
TG+T−T−	(180,070,194,182)	0.000
TTTT	(180,180,180,180)	0.146
G−G−T+T+	(296,293,164,178)	0.687
G−T−T−T	(297,185,182,180)	0.728
T−G−G−T−	(181,299,318,182)	0.822
TTG−T	(180,180,303,180)	0.995
G−g+T−T−	(301,084,207,183)	1.102
G−G−G−T+	(303,306,300,179)	1.216
G−T−G−T	(297,184,303,180)	1.556
G−T−G+T	(297,183,060,180)	1.593
G−G+G+T+	(296,074,043,179)	1.798
TG−T+C−	(180,289,172,358)	8.065
TTTC	(180,180,180,000)	8,144
G−T−TC	(297,184,180,000)	8.726
G−G−T+C−	(296,290,172,358)	8.776
G−g+T−C+	(301,089,191,002)	9.485
T+T−g−C−	(179,183,270,354)	9.744
G−G−g−C−	(302,304,273,352)	9.924
T−G−g−C−	(182,297,275,351)	9.990
G−T−g−C−	(296,185,270,354)	10.264
G−T−g+C+	(298,182,089,007)	10.323
g+G−g−C−	(090,308,276,350)	11.690
G−a+G+C+	(297,097,074,013)	11.960

Table S.2.: All conformers of $(TS_{\alpha'})^{\ddagger}$, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4,\phi_5)$	$U_{j\mathrm{x}}$
TG−T+T+g−	(180,290,167,177,280)	0.000
TG−T+T+g+	(180,290,167,179,080)	0.000
TTT+T+g−	(180,180,179,179,279)	0.111
G−G−T+T+g+	(296,293,165,179,080)	0.671
G−G−T+T+g−	(296,292,165,177,280)	0.680
G−T−T−T−g+	(297,185,182,181,080)	0.688
G−T−TT+g−	(297,184,180,179,279)	0.690
T−G−G−T+g−	(181,300,313,179,279)	0.741
T−G−G−T−g+	(181,299,316,182,080)	0.832
TTG+T−g+	(180,180,064,182,081)	0.960
TTG−T−g+	(180,180,301,181,080)	0.979
G−g+T−T−g−	(301,083,209,181,281)	1.016
G−G−G−T+g−	(302,306,298,177,280)	1.057
G+g−T+T+g−	(059,275,155,176,280)	1.125
G−G−G−Tg+	(302,306,301,180,080)	1.210
G−T−G−T+g−	(297,184,296,178,279)	1.512
G−T−G−T−g+	(297,184,301,181,081)	1.532
G−T−G+T−g+	(297,183,067,182,081)	1.539
G−G+G+Tg+	(295,073,044,180,079)	1.598
G−G+G+T+g−	(296,074,043,178,280)	1.829
TG−T+CG−	(180,289,170,000,288)	6.868
TT−T−C+G+	(180,181,185,001,072)	6.987
TG−T+C+G+	(180,287,179,001,070)	7.074
G−G−T+CG−	(298,291,168,000,288)	7.420
G−T−T−C+G+	(297,184,185,001,072)	7.538
G−T−T+C−G−	(296,183,174,359,288)	7.554
G−G−T+C+G+	(295,288,179,001,070)	7.801
G+g−T+C−G−	(058,272,166,359,288)	8.173
T−T+g+C+G+	(181,177,090,002,071)	8.513
G+a−T+C+G+	(060,269,177,001,069)	8.579
G+G+g+C+G+	(058,056,088,005,070)	8.718
T−G−g−C−G−	(182,297,274,354,290)	8.737
T+T−A−C−G+	(179,183,254,350,065)	8.842
G+T+a+C+G+	(065,175,091,003,071)	9.010
G+T+g−C−G−	(062,178,270,357,289)	9.091
G−G−g−C+g+	(301,311,284,005,087)	9.215
T+G+G+C−g−	(177,044,071,357,273)	9.227
T−T+g+C−g−	(181,176,080,354,271)	9.266
G+G+a+C+G−	(057,058,093,018,291)	9.339
T+G+a+C+G−	(178,066,091,020,291)	9.396
G−T−g+C−g−	(298,181,080,354,271)	9.879
g−G+g+C+G+	(270,051,085,006,070)	10.499
G+a−G−C−G−	(063,263,285,350,291)	10.693
g+G−g−C+g+	(087,305,283,002,090)	10.749
a+G−g−C−G+	(093,306,273,337,071)	11.361
G+a−G−C−G+	(064,266,285,333,070)	11.626

Table S.3.: All conformers of $(TS_\alpha)^\ddagger$, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4)$	$U_{j\mathrm{x}}$
T+G+T−T−	(179,072,195,183)	0.000
T−T−T−T−	(181,188,195,182)	0.308
G+G+T−T−	(063,070,195,183)	0.623
G−g+T−T−	(300,088,199,183)	0.795
G−T−T−T−	(299,194,195,183)	0.846
T+G+C+T+	(179,068,028,178)	0.880
T+G−T−T−	(179,290,186,181)	0.913
T−T−C+T+	(181,183,028,178)	1.071
G+T+T−T−	(062,171,192,182)	1.176
G+G+C+T+	(062,065,030,178)	1.408
G−g+G+T+	(297,080,033,178)	1.552
G−T−C+T+	(296,186,028,178)	1.690
G+T+C+T+	(061,169,027,178)	1.886
G+a−T−T−	(061,266,185,181)	2.101
G−G−T−T−	(308,309,192,182)	2.209
T+g−C+T+	(178,283,015,179)	2.256
G−G−G+T+	(305,305,042,178)	3.506
G+a−C+T+	(064,259,016,178)	3.587
g−g−C+T+	(277,281,018,178)	3.824
TG+T−C+	(180,074,187,002)	8.039
T−T−T−C+	(181,185,186,002)	8.374
G+G+T−C+	(063,072,187,001)	8.703
T+G−T−C+	(178,290,182,004)	8.859
G−T−T−C+	(297,189,186,002)	8.956
G−g+T−C+	(299,090,189,002)	9.099
G+T+T−C+	(062,170,186,003)	9.208
G+a−T−C+	(060,266,183,005)	10.127

Table S.4.: All conformers of $(TS_\beta)^\ddagger$, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4)$	U_{jx}
T+G+T−T−	(177,073,186,181)	0.000
T+T+T+T+	(177,176,165,178)	0.199
G+G+T−T−	(051,069,188,181)	0.644
G+T+T+T+	(053,171,166,178)	0.732
G−T+T+T+	(289,177,164,178)	0.741
T+G+G+T+	(177,067,038,178)	0.768
G+G+a+T−	(050,063,093,183)	0.825
G−g+T−T−	(297,089,199,183)	0.891
T+G+a−T+	(177,072,260,178)	0.945
T+T−G−T−	(178,187,328,181)	1.014
G+G+g−T+	(051,068,271,178)	1.041
T+G−T+T+	(179,299,175,179)	1.050
G−g+G+T+	(291,077,044,179)	1.278
G−T−G−T−	(291,189,326,181)	1.492
G−G−T+T+	(293,301,172,178)	1.629
G+T−G−T−	(053,182,326,181)	1.679
TG−G−T−	(180,311,313,182)	1.733
G−G−G−T+	(298,316,295,179)	1.905
G−G−a+T−	(295,308,095,182)	2.343
G+G−G−T+	(061,299,308,179)	3.024
G+G−T+T+	(052,285,152,177)	3.037
G+A−G+T−	(060,242,073,184)	3.988
T+G+T−C+	(177,075,184,001)	8.033
T+T+T+C−	(177,176,173,357)	8.510
G+G+T−C+	(050,070,184,001)	8.672
G+T+T+C−	(052,171,173,357)	9.052
G−T+T+C−	(288,176,172,357)	9.063
G−a+T−C+	(296,093,187,002)	9.089
G+G+g+C+	(051,061,089,007)	9.346
T+G+g+C+	(178,069,089,007)	9.346
TG−T+C	(180,297,177,000)	9.498
G−G−a−C−	(298,309,262,356)	10.008
G−G−T+C	(293,299,176,000)	10.061
T−G−a−C−	(181,302,262,355)	10.120
a−G+g+C+	(267,055,085,008)	10.511
G−a+g+C+	(292,104,077,012)	10.782
T+Tg−C−	(177,180,279,349)	10.887
G−T+g−C−	(285,169,281,348)	11.287
G+T+g−C−	(052,174,280,349)	11.392
T+G−a+C+	(174,305,105,003)	11.590
G+a−g−C−	(057,262,282,353)	11.703
G+g−T+C−	(054,278,173,358)	11.818
g+G−a−C−	(081,328,265,359)	11.921

Table S.5.: All conformers of $(TS_\gamma)^\ddagger$, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4)$	U_{jx}
T+G+T−T−	(177,070,189,181)	0.000
T+T+T+T	(176,179,179,180)	0.293
G−G−T+T+	(294,293,167,178)	0.805
G+g−T+T+	(051,278,160,177)	0.924
G+T+TT	(055,175,180,180)	0.951
G−T−TT	(291,181,180,180)	1.021
T−G−G−T+	(183,297,304,178)	1.196
T+g−A+T+	(171,281,144,179)	1.228
T+G+G+T+	(178,064,034,178)	1.271
G+G+G+T−	(046,058,064,183)	1.317
G−g+T−T−	(293,080,206,183)	1.335
T+T+G+T+	(176,179,046,179)	1.335
T+T+G−T−	(176,179,315,181)	1.456
G−G−G−T+	(300,305,297,179)	1.461
G+G+A−T+	(050,064,253,177)	1.571
G−G+G+T−	(286,067,049,181)	1.728
G−T−G−T	(292,181,303,180)	1.796
G−T−G+T	(291,181,058,180)	1.807
G+T+G−T−	(055,177,309,181)	1.991
G+G−G−T−	(052,285,323,182)	2.041
T+G+T−C+	(176,071,187,002)	7.834
T+T+T+C−	(175,179,177,358)	8.178
G+T+T−C+	(057,177,183,001)	8.867
G−G−T+C−	(295,292,174,359)	8.934
G+g−T+C−	(052,275,170,358)	8.961
G−T−TC	(291,181,180,000)	9.084
G−g+T−C+	(291,084,191,001)	9.723
T+T−g+C+	(179,185,087,008)	9.760
T+g−T+C−	(164,275,168,357)	9.972
G−G−g−C−	(299,304,272,353)	10.126
A+G−T+C−	(125,290,170,355)	10.165
G+T+g−C−	(052,171,274,352)	10.267
TG+g+C+	(180,067,087,008)	10.364
T+T−g−C−	(175,181,270,354)	10.487
g+g+T−C+	(078,084,191,004)	10.497
G−T+g+C+	(292,178,090,006)	10.713
G−T−g−C−	(291,183,270,353)	10.746
G+T+a+C+	(057,175,091,006)	11.138
T−G−g−C−	(192,309,274,354)	11.165
a−G+g+C+	(268,056,085,010)	11.267
G+a−G−C−	(055,266,285,347)	12.221

Table S.6.: All conformers of $(TS_\delta)^\ddagger$, the torsional angles, and the difference in energy between them (in kcal/mol).

Structures	$(\phi_1,\phi_2,\phi_3,\phi_4,\phi_5)$	U_{jx}
TG−T+T+G+	(180,290,168,178,062)	0.000
TG−T+T+T+	(180,290,167,178,179)	0.320
G−G−T+T+g+	(303,296,169,179,077)	0.332
TTTTT	(180,180,180,180,180)	0.452
T−G−T+T+G−	(184,291,168,178,299)	0.453
T+T+T+T+G−	(179,178,176,179,296)	0.478
G+g−T+TG−	(063,274,168,180,287)	0.491
G−T−TTg+	(298,185,180,180,076)	0.656
G−G−T+T+G−	(296,293,167,178,300)	0.683
G−G−T+T+T−	(297,292,165,178,186)	0.910
G−T−T−TT−	(297,184,181,180,187)	0.928
TG−G−T−G+	(180,298,319,182,062)	1.008
G−T−T−T−G−	(297,187,185,181,301)	1.076
T−G−G−T−G−	(182,299,318,181,297)	1.109
G+g−T+T+T+	(059,279,152,177,173)	1.150
T−G−G−T−T	(181,298,320,182,180)	1.265
TTG−T−G−	(180,180,309,181,297)	1.333
T+T−G−TG+	(179,181,306,180,063)	1.336
TTG−TT	(180,180,304,180,180)	1.363
G−G−G−T+G−	(305,307,299,179,307)	1.417
G+G+G+T−T+	(057,054,061,181,174)	1.532
G−T−G−Tg+	(298,184,304,180,077)	1.656
G−T−G+Tg+	(300,184,063,180,077)	1.710
G−G+G+T+T−	(295,071,046,179,189)	1.765
G−T−G−TT−	(297,183,306,180,188)	1.806
G−G+G+T−G−	(297,075,047,182,304)	1.869
G−T−G+TT−	(297,183,057,180,187)	1.876
G−G−C−T−g+	(298,297,331,182,077)	1.894
G−T−G−TG−	(296,184,306,180,300)	1.973
G−T−G+T+G−	(295,183,053,179,299)	1.992
G+g−A+T+G+	(060,274,150,177,061)	2.148
G+g−C−T−G−	(069,277,344,181,288)	2.599
G−G−T+C−G+	(302,295,168,356,075)	7.839
TG−T+C−G+	(180,289,173,358,062)	8.044
G+g−T+C−G−	(060,273,168,354,287)	8.150
G−T−T+C−g+	(299,185,179,359,076)	8.266
TG−T+C−T+	(180,289,172,358,178)	8.430
TTTCT	(180,180,180,000,180)	8.483
T−T−T−C+G+	(181,182,182,001,065)	8.571
T−G−T+C−G−	(184,290,173,358,299)	8.613
G−G−T+C−G−	(296,291,173,359,301)	8.785
G−T−TCT−	(297,184,180,000,187)	8.981
G−G−T+C−T−	(297,290,173,359,188)	9.067
G−T−T−C+G−	(297,186,182,001,302)	9.209
G−g+T−C+T−	(300,086,192,001,186)	9.603
G+G+g+C+G+	(055,056,088,008,048)	9.993
T−T−g−C−G+	(181,183,271,354,064)	10.004
T−G−g−C−G+	(181,297,274,351,062)	10.085
T+G+g+C+G+	(177,061,086,008,062)	10.093
G−T−g−C−G−	(304,186,271,353,314)	10.169

T−T+g+C+T	(181,177,090,006,180)	10.226
G−G−g−C−T−	(303,304,272,352,189)	10.242
TT+g+C+G+	(180,178,089,006,063)	10.352
G+T+a+C+g−	(063,173,092,005,284)	10.374
G−T−g+C+g+	(301,182,090,006,077)	10.378
G−g+T−C+G−	(295,090,189,002,297)	10.560
T+G+g+C+T−	(179,063,086,009,181)	10.610
G+T+g+C+T+	(064,175,090,006,174)	10.678
G−Tg+C+T−	(298,180,090,006,187)	10.716
G−T−g+C+G−	(296,182,088,007,298)	11.031
G+G+g+C+G−	(069,065,089,007,287)	11.207
g−G+g+C+G−	(272,051,083,010,298)	11.443
g+G−g−C−T+	(085,307,277,351,170)	11.785
G−a+G+C+G−	(296,096,075,011,299)	12.154

Table S.7.: Forward classical barriers ($V^{\ddagger}$) for ($R_{\alpha'}$)-(R_{δ}), obtained at the theory level DLPNO-CCSD(T)-F12. All values in kcal/mol.

Reactions	cc-pVDZ-F12	cc-pVTZ-F12	cc-pVQZ-F12	CBS$_{D-Q}$
($R_{\alpha'}$)	11.90	12.11	12.04	11.99
(R_{α})	8.70	8.85	8.80	8.76
(R_{β})	9.75	9.90	9.80	9.73
(R_{γ})	9.09	9.16	9.02	8.92
(R_{δ})	11.52	11.58	11.52	11.48

Table S.8.: MS-CVT/SCT rate constants for ($R_{\alpha'}$)-(R_{δ}), including all conformations of methyl pentanoate and transition states.

T(K)	($R_{\alpha'}$)	(R_{α})	(R_{β})	(R_{γ})	(R_{δ})
200	1.28E-19	5.42E-17	1.31E-17	2.44E-17	1.09E-19
298	1.51E-17	1.32E-15	6.61E-16	1.01E-15	2.04E-17
300	1.62E-17	1.38E-15	6.99E-16	1.06E-15	2.21E-17
500	3.11E-15	4.74E-14	4.47E-14	5.41E-14	5.60E-15
750	8.34E-14	4.70E-13	5.90E-13	6.04E-13	1.55E-13
1000	5.66E-13	1.90E-12	2.68E-12	2.47E-12	1.03E-12
1100	9.99E-13	2.92E-12	4.20E-12	3.77E-12	1.79E-12
1150	1.29E-12	3.54E-12	5.15E-12	4.56E-12	2.30E-12
1200	1.63E-12	4.24E-12	6.23E-12	5.44E-12	2.89E-12
1250	2.04E-12	5.03E-12	7.44E-12	6.43E-12	3.60E-12
1300	2.52E-12	5.91E-12	8.80E-12	7.52E-12	4.41E-12
1350	3.06E-12	6.88E-12	1.03E-11	8.73E-12	5.34E-12
1400	3.69E-12	7.96E-12	1.20E-11	1.00E-11	6.39E-12
1450	4.39E-12	9.13E-12	1.38E-11	1.15E-11	7.57E-12
1500	5.19E-12	1.04E-11	1.58E-11	1.30E-11	8.90E-12
1550	6.08E-12	1.18E-11	1.79E-11	1.47E-11	1.04E-11
1600	7.06E-12	1.33E-11	2.03E-11	1.64E-11	1.20E-11
1650	8.15E-12	1.49E-11	2.28E-11	1.83E-11	1.38E-11
1700	9.33E-12	1.66E-11	2.54E-11	2.04E-11	1.57E-11
1800	1.20E-11	2.04E-11	3.13E-11	2.48E-11	2.01E-11
1900	1.52E-11	2.46E-11	3.80E-11	2.97E-11	2.52E-11
2000	1.89E-11	2.93E-11	4.54E-11	3.51E-11	3.10E-11
2500	4.50E-11	6.03E-11	9.35E-11	6.99E-11	7.19E-11
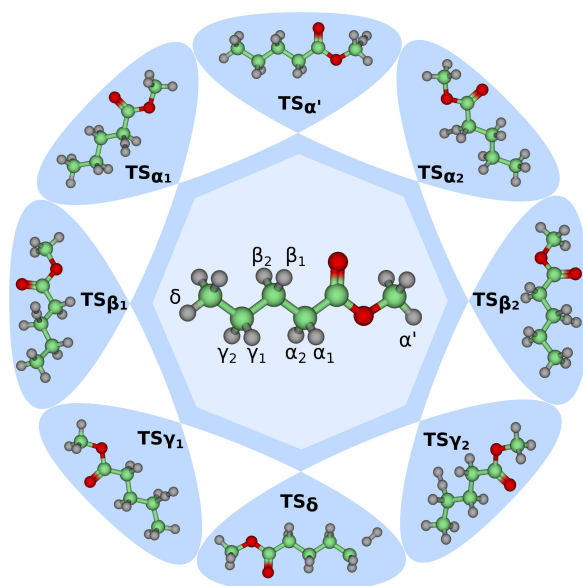
Fig. S.1.: Three-dimensional representation of methyl pentanoate (MP) and transition states generated by the reactions $(R_{\alpha'})$–(R_{δ}).
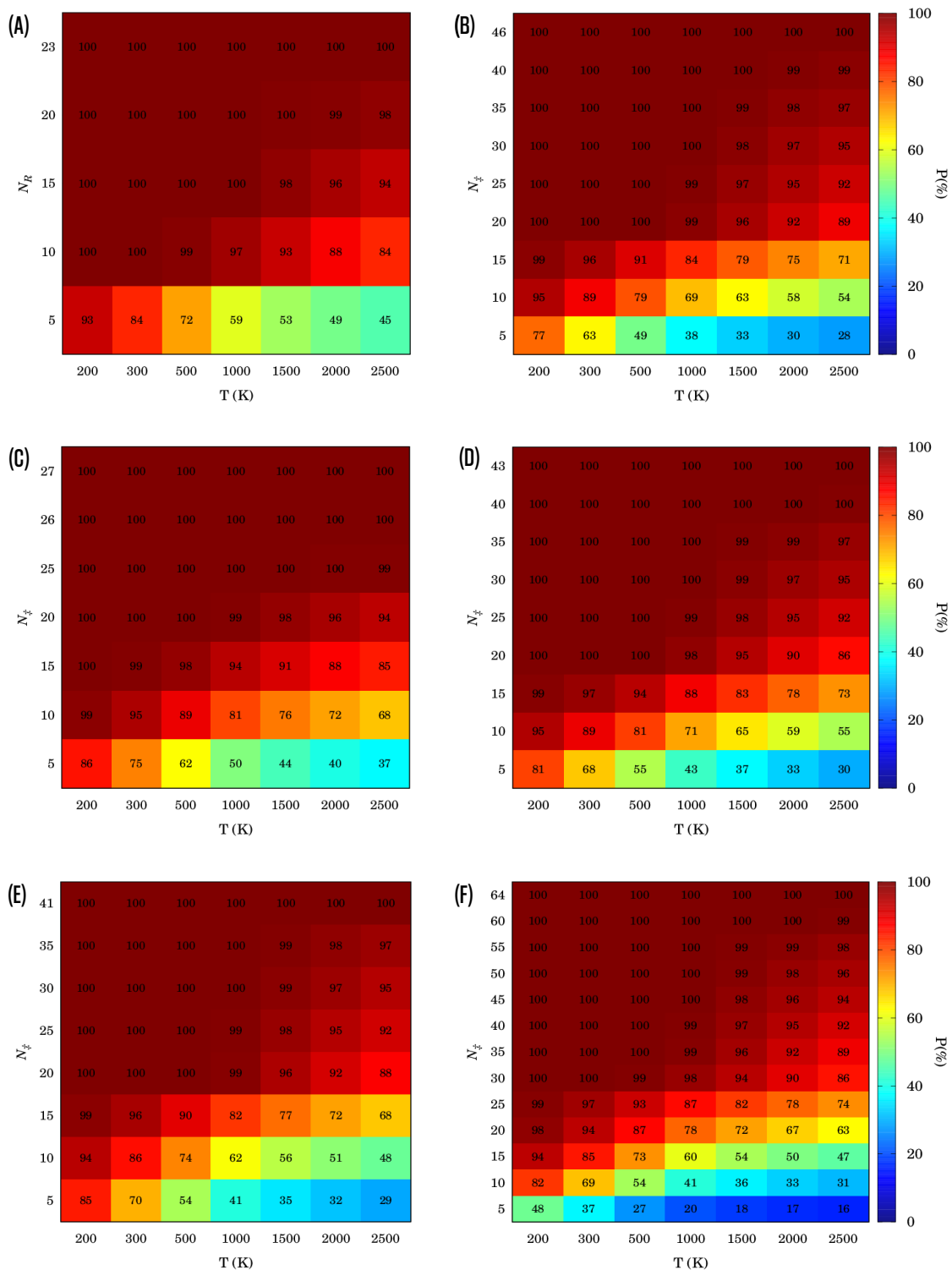
Fig. S.2.: Heatmaps plots show the truncation efficiency on the rovibrational partition function, as a function of the temperature, for MP (A), $(TS_{\alpha'})^{\ddagger}$ (B), $(TS_{\alpha})^{\ddagger}$ (C), $(TS_{\beta})^{\ddagger}$ (D), $(TS_{\gamma})^{\ddagger}$ (E), and $(TS_{\delta})^{\ddagger}$ (F).
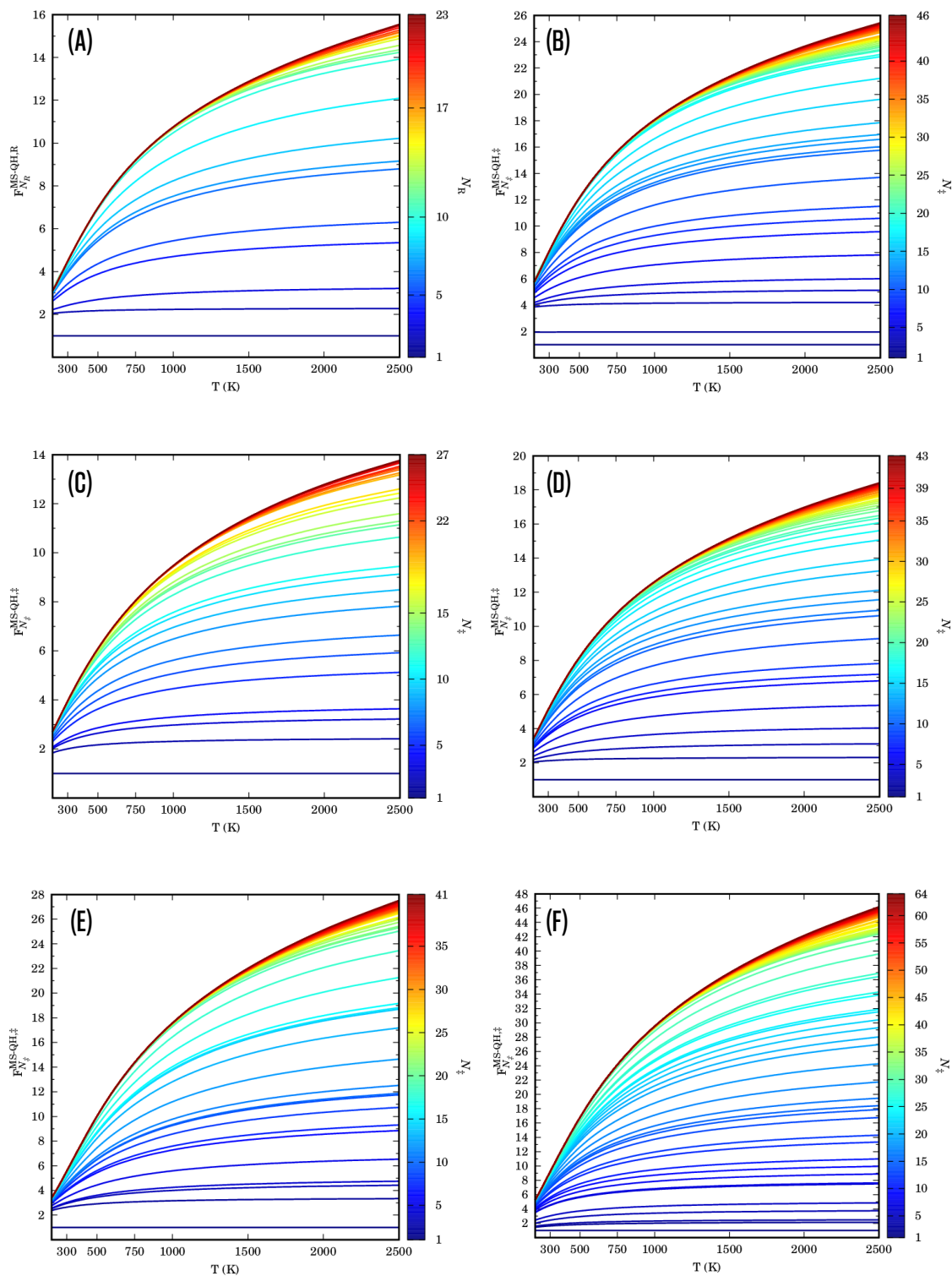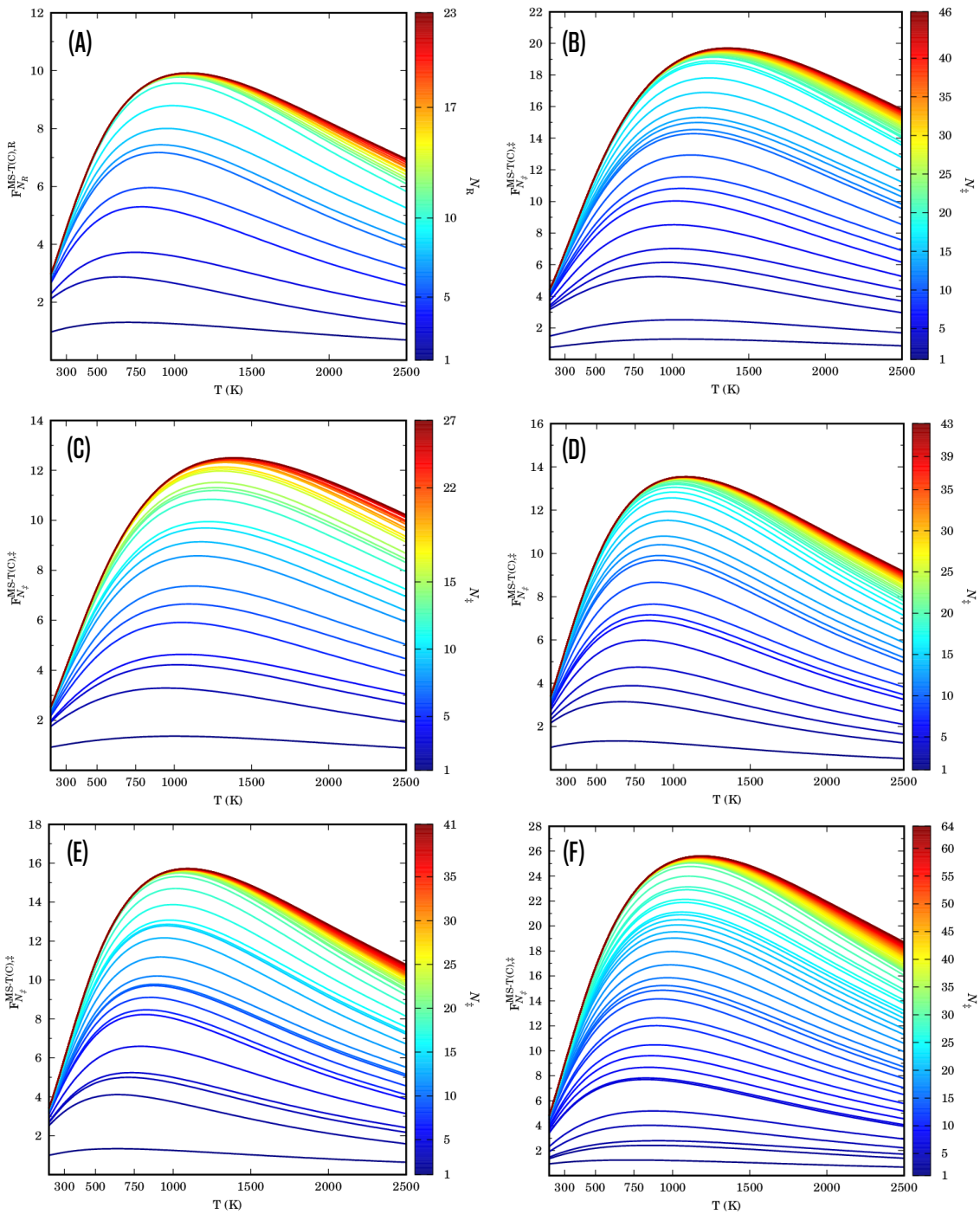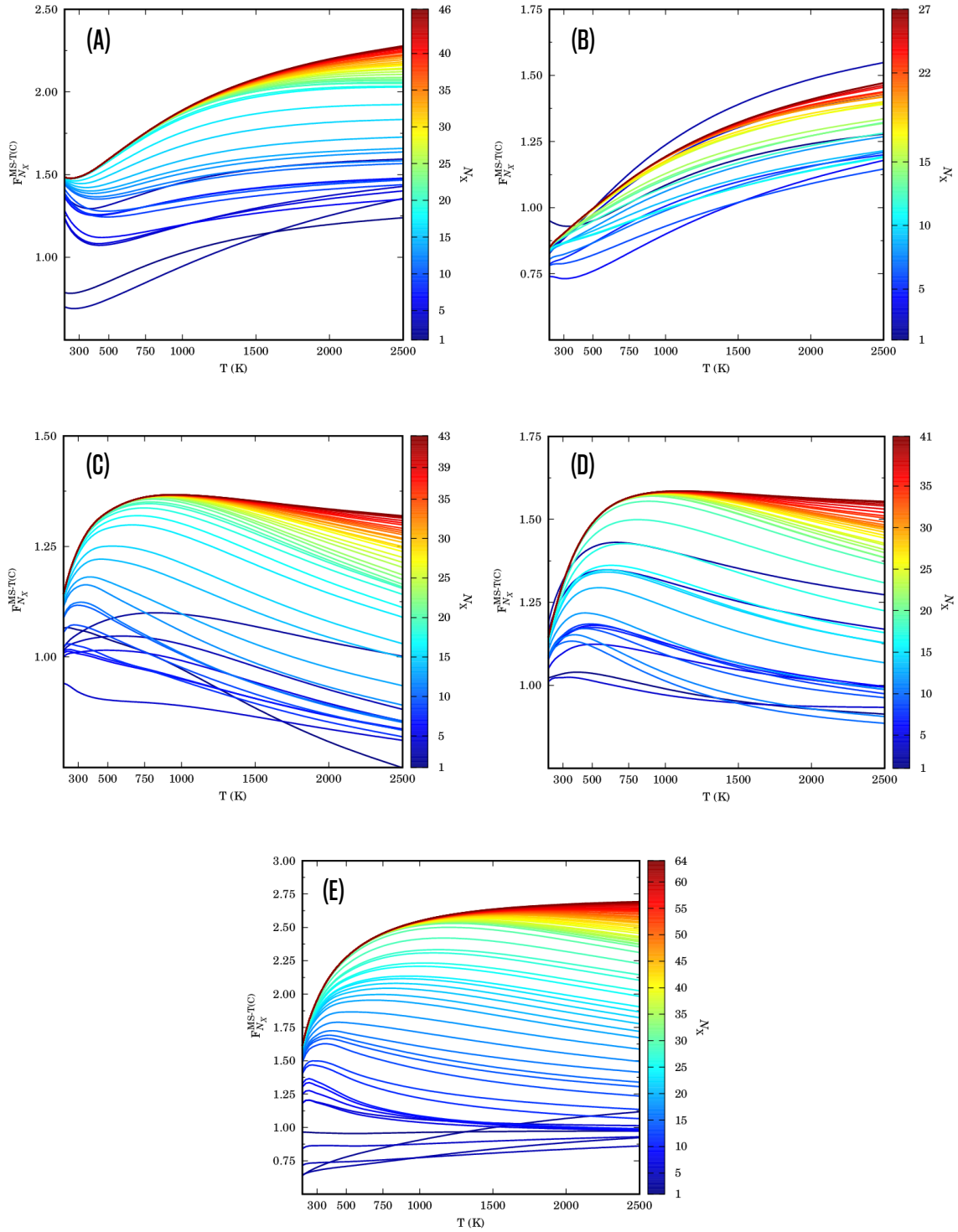
Fig. S.3.: Multistructural factors $(F_{N_X}^{\mathrm{MS\text{-}QH,X}})$ as a function of temperature and different sets of conformers, for MP (A), $(\mathrm{TS}_{\alpha'})^{\ddagger}$ (B), $(\mathrm{TS}_{\alpha})^{\ddagger}$ (C), $(\mathrm{TS}_{\beta})^{\ddagger}$ (D), $(\mathrm{TS}_{\gamma})^{\ddagger}$ (E), and $(\mathrm{TS}_{\delta})^{\ddagger}$ (F).
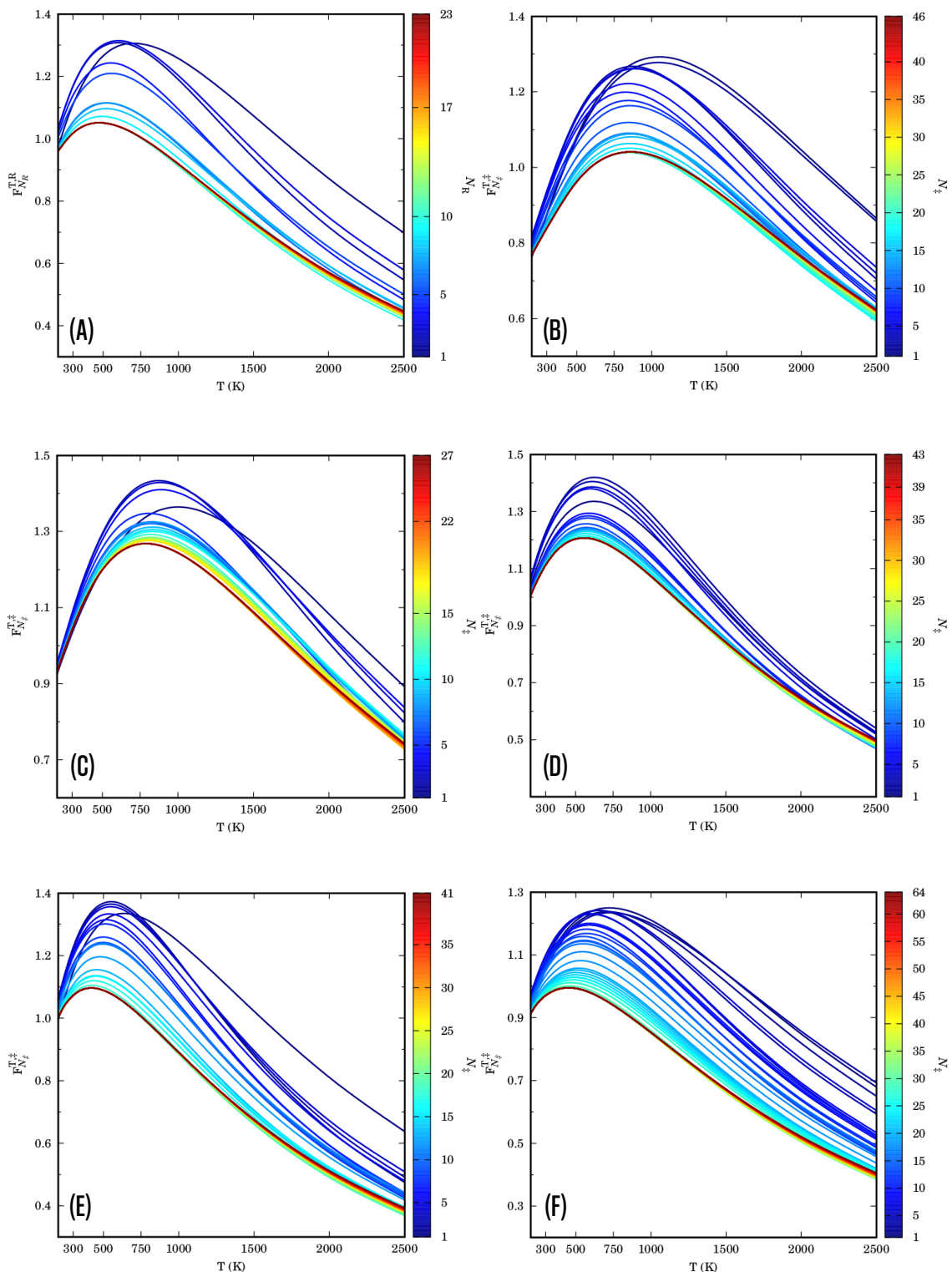
Fig. S.4.: Torsional anharmonic factors $(F_{N_X}^{\mathrm{T,X}})$ as a function of temperature and different sets of conformers, for MP (A), $(\mathrm{TS}_{\alpha'})^{\ddagger}$ (B), $(\mathrm{TS}_{\alpha})^{\ddagger}$ (C), $(\mathrm{TS}_{\beta})^{\ddagger}$ (D), $(\mathrm{TS}_{\gamma})^{\ddagger}$ (E), and $(\mathrm{TS}_{\delta})^{\ddagger}$ (F).

Fig. S.5.: Individual multistructural torsional anharmonic factors ($F_{N_X}^{MS-T,X}$) as a function of temperature and different sets of conformers, for MP (A), $(TS_{\alpha'})^{\ddagger}$ (B), $(TS_{\alpha})^{\ddagger}$ (C), $(TS_{\beta})^{\ddagger}$ (D), $(TS_{\gamma})^{\ddagger}$ (E), and $(TS_{\delta})^{\ddagger}$ (F).

Fig. S.6.: Multistructural torsional anharmonic factor $(F_{N_X}^{\text{MS-T}})$, as a function of temperature and different sets of conformers. $(\text{R}_{\alpha'})$ (A), (R_{α}) (B), (R_{β}) (C), (R_{γ}) (D), and (R_{δ}) (E).
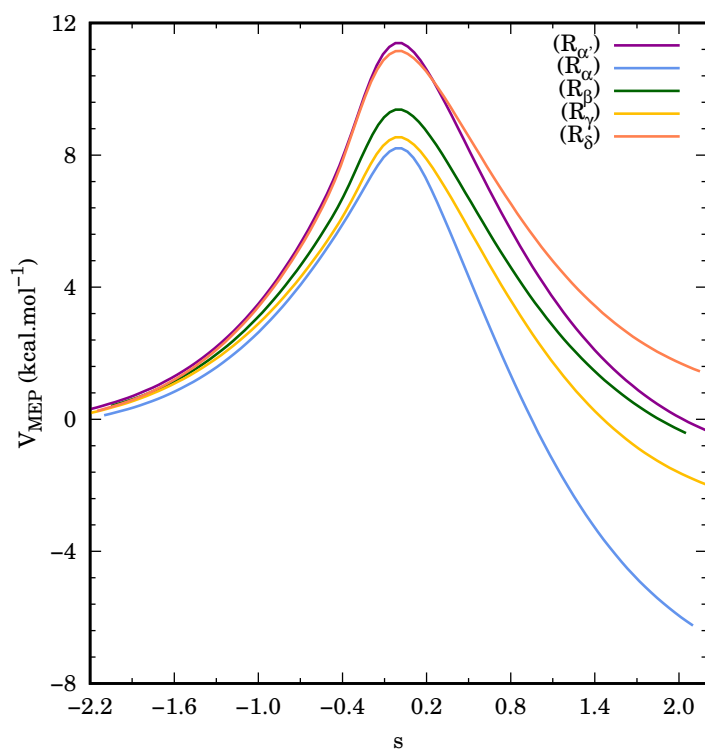
Fig. S.7.: Minimum energy path (V_{MEP}), in kcal/mol, obtained at MPWB1K/6-31+G(d,p) theory level.
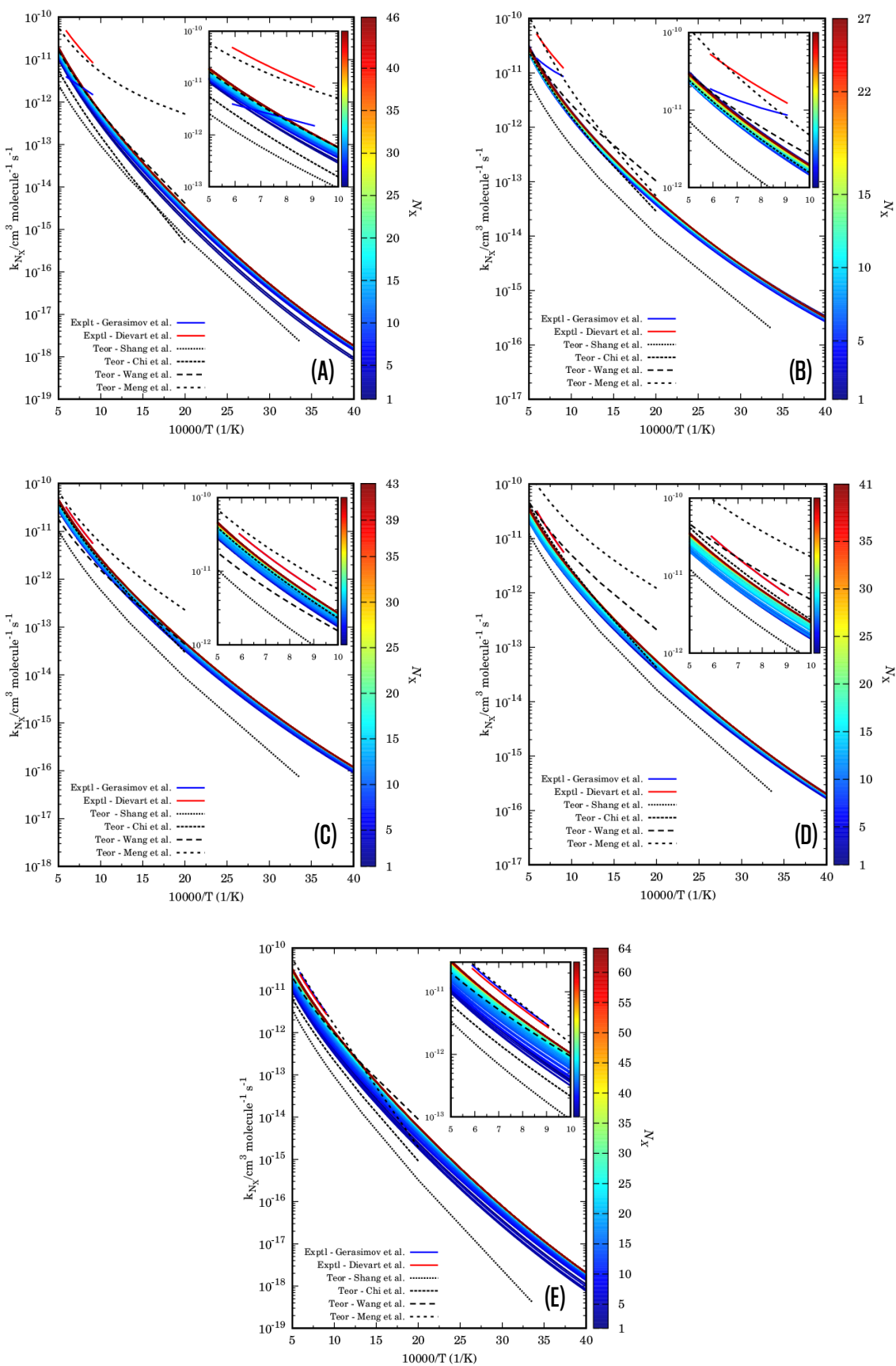
Fig. S.8.: Arrhenius plots showing MS-CVT/SCT rate constants, as a function of conformational set. Theoretical and experimental values are also showed. ($R_{\alpha'}$) (A), (R_α) (B), (R_β) (C), (R_γ) (D), and (R_δ) (E).
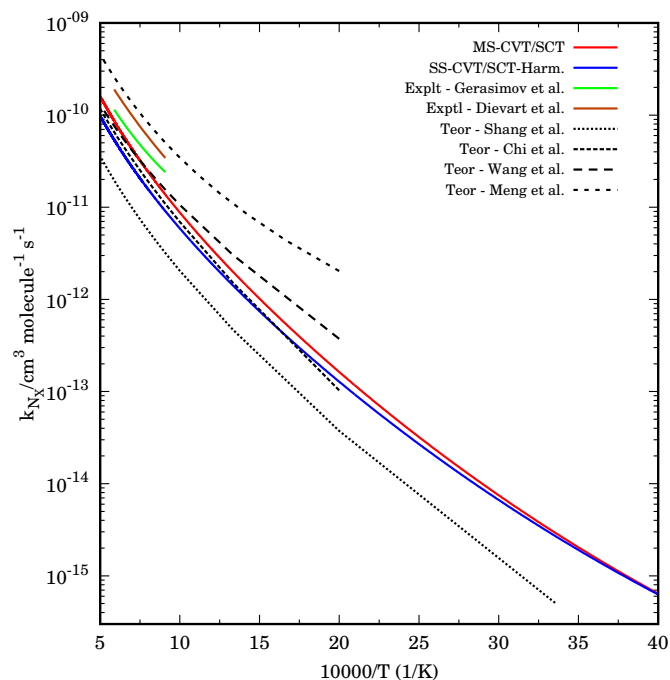
Fig. S.9.: Arrhenius plots showing overall MS-CVT/SCT and SS-CVT/SCT rate constants, as a function of temperature. Theoretical and experimental values are also showed.
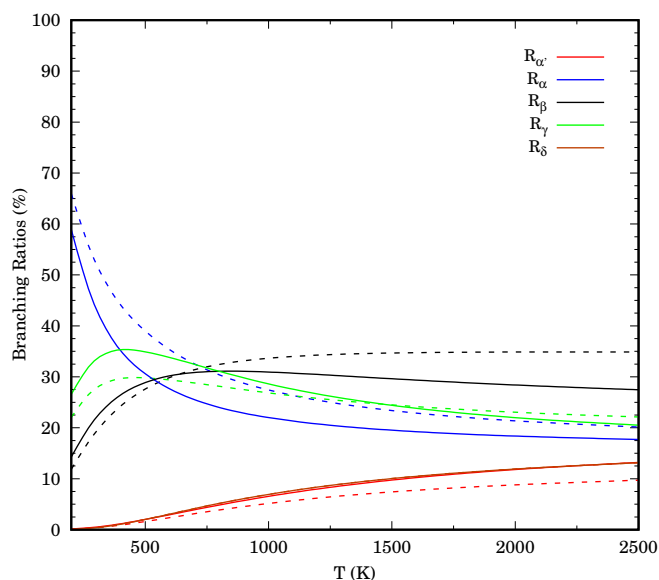
Fig. S.10.: Branching ratios for $(R_{\alpha'})$-(R_{δ}), calculated by ratio between the individual and the total rate constants. Solid line: obtained from MS-CVT/SCT rate constants. Dashed line: obtained from SS-CVT/SCT rate constants.
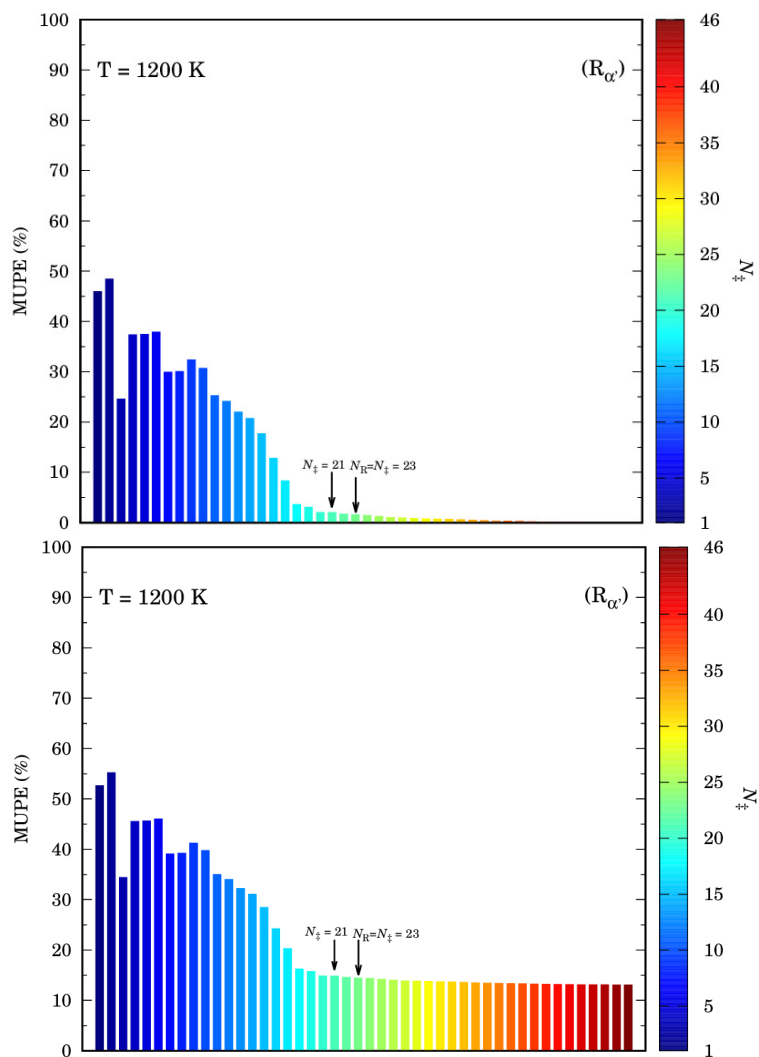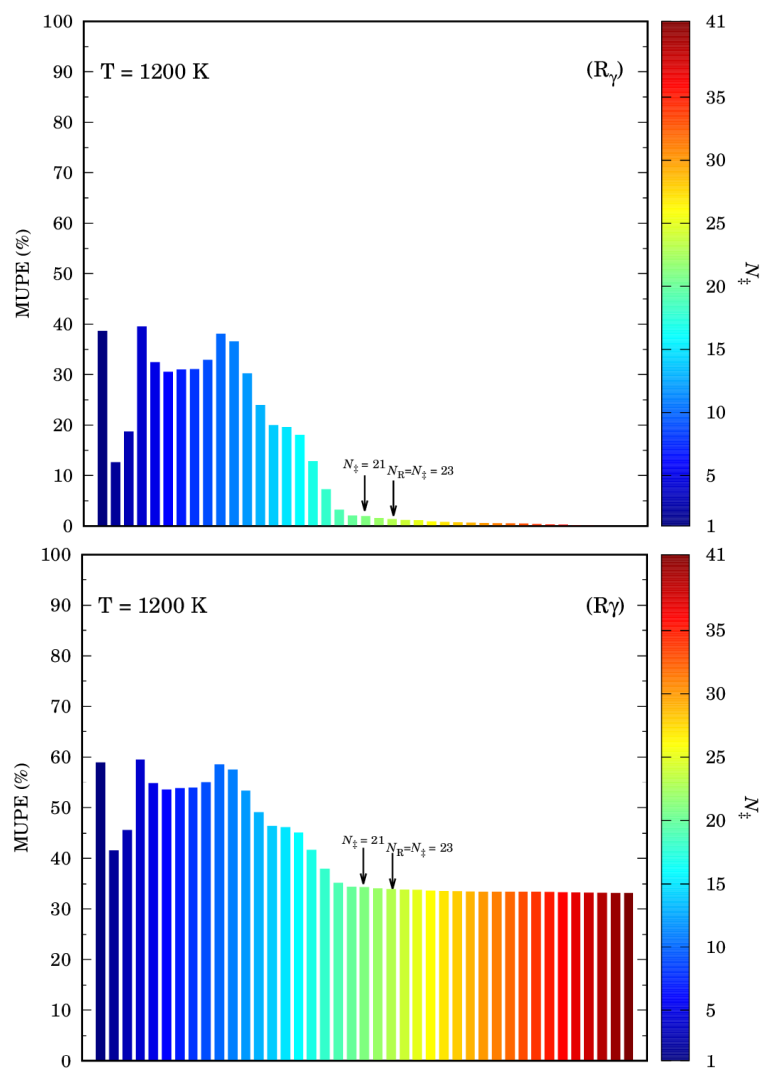
Fig. S.11.: Mean Unsigned Percentage Error (MUPE) of truncated thermal rate constants estimative, at 1200 K, comparaed to the full MS-CVT/SCT results (top) and Gerasimov et al. findings (bottom) for ($R_{\alpha'}$).
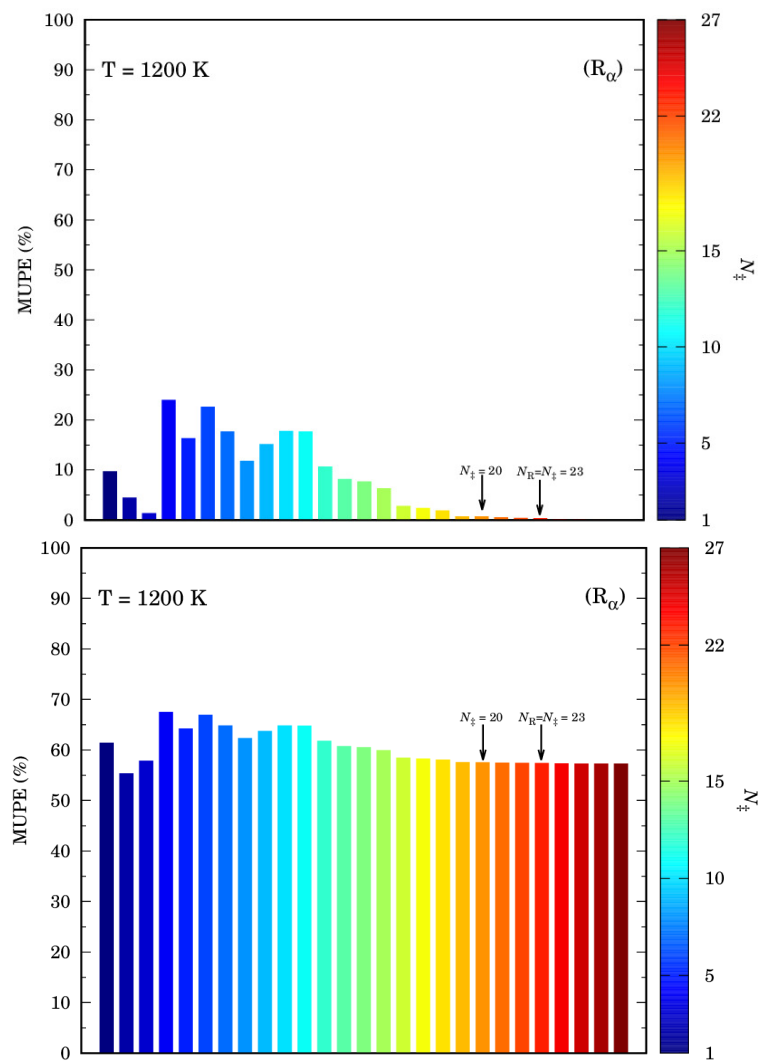
Fig. S.12.: Mean Unsigned Percentage Error (MUPE) of truncated thermal rate constants estimative, at 1200 K, comparaed to the full MS-CVT/SCT results (top) and Gerasimov et al. findings (bottom) for (R_α).
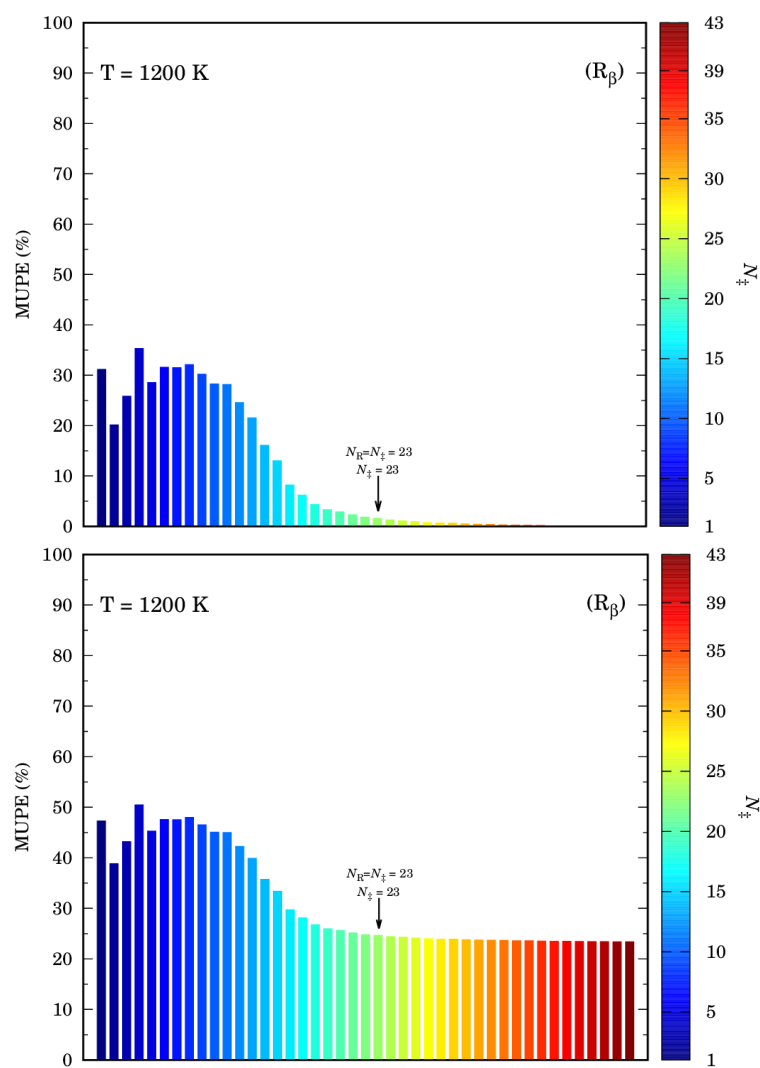
Fig. S.13.: Mean Unsigned Percentage Error (MUPE) of truncated thermal rate constants estimative, at 1200 K, comparaed to the full MS-CVT/SCT results (top) and Gerasimov et al. findings (bottom) for (R$_\beta$).

Fig. S.14.: Mean Unsigned Percentage Error (MUPE) of truncated thermal rate constants estimative, at 1200 K, comparaed to the full MS-CVT/SCT results (top) and Gerasimov et al. findings (bottom) for (R_γ).
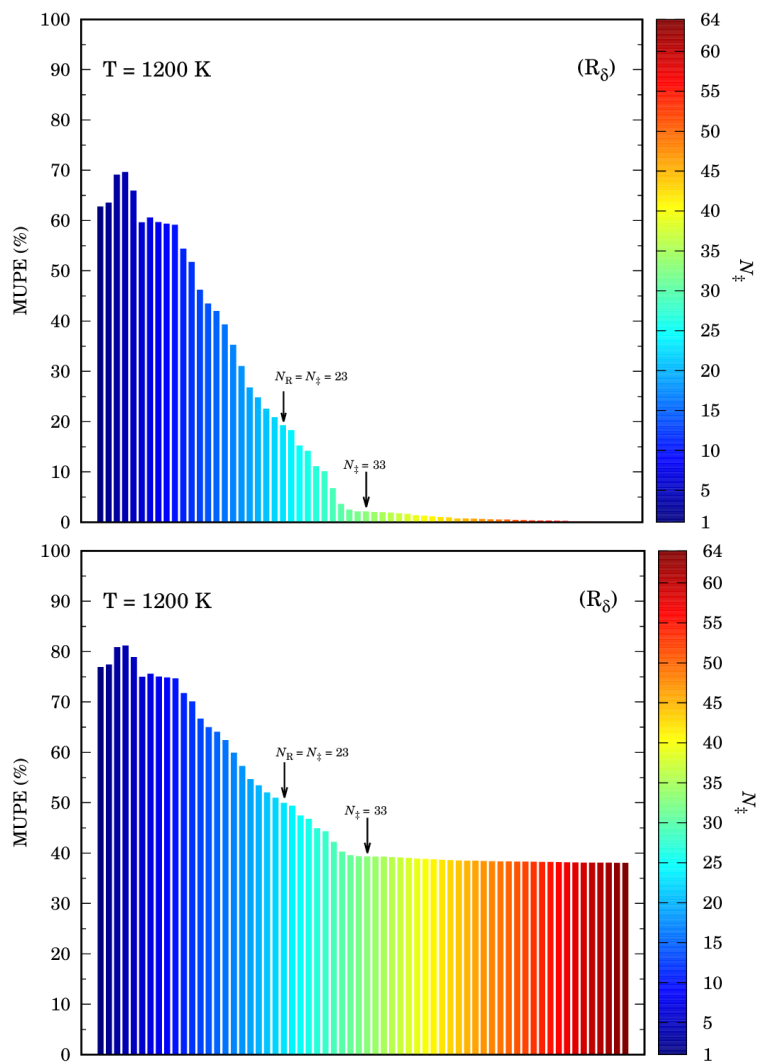
Fig. S.15.: Mean Unsigned Percentage Error (MUPE) of truncated thermal rate constants estimative, at 1200 K, comparaed to the full MS-CVT/SCT results (top) and Gerasimov et al. findings (bottom) for (R_δ).