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DFT and experimental study of triallylborane-mediated isomerization of α-allylated azaheterocycles

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Table of Contents:

Experimental section

General: All reactions and manipulations with triallylborane were carried out under inert atmosphere of dry argon. NMR spectra were recorded on Bruker Avance-400 MHz instrument. All solvents and reagents were purified using standard methods. Triallylborane was prepared by the Zakharkin and Stanko method[S1]. *trans*-Isomers **2a**[S2], **2b**[S3], **2c**[S4] and **2d**[S5] were synthesized as described.

The *trans/cis*-isomerization of α-allylated heterocycles **2a-c** was carried out in accordance with described procedures as following:

Isomerization of *trans*-2,6-diallyl-1,2,3,6-tetrahydropyridine 2a to *cis*-2a.[S2]

To a degassed **2a** (5.9 g, 36.2 mmol) under Ar atmosphere was added triallylborane (5.4 g, 6.9 ml, 40.3 mmol) with stirring and the mixture was heated at 135 °C for 15 h. After the isomerization was completed (^{1}H NMR control of an aliquot of the deboronated reaction mixture), the mixture was treated successively with MeOH (5 ml) and 20% NaOH (25 ml) and heated under reflux for 1 h. The cooled two-phase mixture was diluted with *n*-hexane (20 ml), the organic layer was separated, washed with brine, dried with K_2CO_3 and evaporated under reduced pressure to give crude ***cis*-2a** (5.6 g, 95%), which was analyzed by ^{1}H NMR that showed the ratio ***cis*-2a**/**2a** = 99:1 by integration of signals (CHN) at 2.80 (***cis*-2a**) and 2.93 (**2a**) ppm.

Isomerization of 1,3-diallyl-1,2,3,4-tetrahydroisoquinoline 2b to *cis*-2b.[S3]

To a degassed **2b** (9.5 g, 46.8 mmol) under Ar atmosphere was added triallylborane (8.4 ml, 6.7 g, 50 mmol) with stirring and the mixture was heated at 135 °C for 2 h. After being cooled the reaction mixture was quenched with MeOH (20 ml) and heated under reflux for 1 h. In order to complete deboronation, 20%

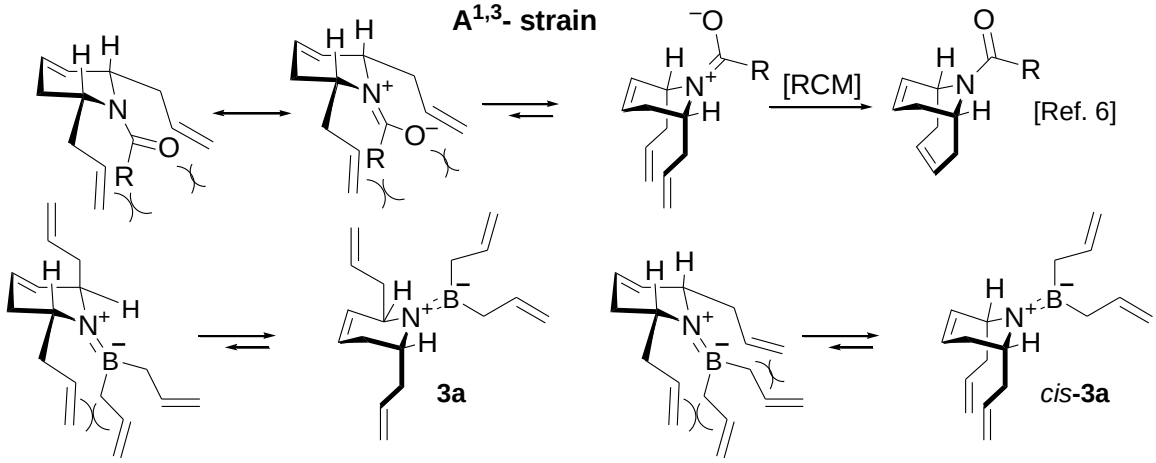
NaOH (30 ml) was added with stirring, and the organic layer was diluted with hexane (30 ml) and separated, dried with K_2CO_3, filtered. Evaporation under reduced pressure gave 9.1 g (96%) of a 1:1 mixture of ***cis*-2b**/**2b** [^{1}H NMR data, integration of CHN signals at 4.07 (***cis*-2b** + **2b**) and 3.15 (**2b**) ppm and also NH at 2.07 (**2b**); 1.87 (***cis*-2b**) ppm].

Isomerization of 3-allyl-1-vinyl-1,2,3,4-tetrahydroisoquinoline 2c to *cis*-2c.[S4]

To a degassed compound **2c** (1.28 g, 6.4 mmol) under Ar atmosphere was added triallylborane (0.95 g, 1.22 ml, 7.0 mmol) with stirring, and the mixture was heated at 175 °C for 9 h. On cooling, the mixture was treated with MeOH (2 ml) and, after gas evolution ceased, with 20% NaOH (3 ml). The mixture was refluxed for 30 min. The product was extracted with ether—hexane (3×5 ml). The combined extracts were dried over K_2CO_3 and concentrated under reduced pressure to give a mixture of ***cis*-2c**/**2c** (1.15 g, 90%), which was analyzed by ^{1}H NMR that showed the ratio ***cis*-2c**/**2c** = 1.54:1 by integration of signals (CHN) at 3.23 (**2c**) and 3.09 (***cis*-2c**) ppm.

Izomerization-exchange reaction of *trans*-2,6-dimethallyl-1,2,3,6-tetrahydropyridines 2d [S5] **with triallylborane.**

To a degassed **2d** (2.12 g, 11.0 mmol) under Ar atmosphere was added triallylborane (1.61 g, 2.08 ml, 12.0 mmol), and the mixture was stirred at 110 °C for 1 h. A small aliquot of the reaction mixture was taken, treated with MeOH, 20% NaOH and analyzed by ^{1}H NMR where signals from CH= and CHN groups of ***cis*-2a** (~15%) were detected. The heating of the aminoborane was continued for 6 h. After treatment content of ***cis*-2a** was about 25%. Such isomerization-exchange process was repeated 4 times when content of ***cis*-2a** was reached about 85%.



Scheme S1. 1,3-Allylic strain in *N*-acyl-piperidines (application for RCM[S6]) and aminoboranes

Geometry optimization and calculation of lowest-free-energies of aminoaboranes

Preliminary optimization of geometry of aminoboranes **3a-c**, ***cis*-3a-c**, **3d, *cis*-3d, *cis*-3''a, *cis*-3-3'''e** were performed with AM1 method, further optimization was done at B3LYP/6-31+G(d,p) level of theory in the Gaussian09 D.01 program package [S7]. Structural guesses for the optimized molecules were generated with Macro Model with coordinates of B, N and all adjacent atoms frozen (plane fragment). Low-energy conformers with relative energies within 5 kcal mol^{-1} having staggered conformations were selected from the conformational search results and optimized at B3LYP/6-31+G(d,p)/PCM(DMSO) level of theory. Harmonic frequencies were calculated to ensure the types of located stationary points and to calculate free energies at experimental temperature 408K (135 °C) for ***cis*-3a**,**b/3a**,**b**; 448K (175 °C) for ***cis*-3c/3c**; 383 K (110 °C) **3d/*cis*-3d, *cis*-3''a**, ***cis*-3-3'''e**. The lowest-free-energies conformations were used to compute isomers ratios (Table 1 and Schemes 1, 3) by formula:

$$K = e^{-\frac{\Delta G}{RT}}$$

K – Equilibrium constant corresponding isomers' ratio; ΔG – difference of free energies of isomers; R – gas constant 0.001987 kcal $(mol*K)^{-1}$; *T* – temperature in Kelvins

Search for transition states of *trans/cis*-isomerization of aminoboranes 3a/*cis*-3a

On the first step, we performed a conformational search for each transition state (TS) (**$TS_{trans\text{-}6}$**, **$TS_{cis\text{-}6}$**, **$TS_{trans\text{-}2}$**, **$TS_{cis\text{-}2}$**) in Macro Model program package using Monte-Carlo/Low-Mode Molecular Dynamics algorithm. The search employed OPLS3 force field, method "Optimal" and a series of constraints:

- Torsion angles C6-N1-B10-C14 and C2-N1-B10-C15 were constrained to 180° (Figure S1).
- For **$TS_{trans\text{-}6}$** and **$TS_{cis\text{-}6}$**:
  - Distances C6-C7 and C9-B10 were constrained to be 2.0Å (we consider this value to be close to the distance in TS).
  - Torsion angle H-C11-C12-C13 was constrained to be 0° (to reduce the number of high energy conformations).
- For **$TS_{trans\text{-}2}$** and **$TS_{cis\text{-}2}$**:
  - Distances C2-C11 and C13-B10 were constrained to be 2.0Å.
  - Torsion angle H-C7-C8-C9 was constrained to be 0°.

Conformational search revealed 147 unique ($RMSD_{no\text{-}hydrogen}$> 0.5Å) structures, which were then pre-optimized in Gaussian09 D.01at B3LYP/6-31+G(d,p)/PCM(DMSO) level of theory with constrained C6-C7 and C9-B10, or C2-C11 and C13-B10 distances (same as in conformational search) and used as initial structures for transition state searches at the same level of theory. Finally, harmonic frequencies of all 147 located transition states were calculated the same level of theory to ascertain their type and calculate vibrational correction to the energies.

All located transition states were clusterized and from each cluster (with$RMSD_{no\text{-}hydrogen}$<0.1Å and Energy difference <0.01 kcal mol^{-1}) only one unique conformer was retained, thus leaving 88 unique conformers (Figure S3).

Intrinsic reaction coordinates were calculated for each unique transition state and their side points were used as initial structures for **3a**, **4a**, **4'a** and ***cis*-3a** searches (Figure S2).

Calculation of contributions to the reaction flow using the Curtin – Hammett principle

The Curtin – Hammett principle in its modern sense states, that the rate (and so, the efficacy) of a particular reaction path is determined by relative energies of the corresponding TSs, assuming that the rate of interconversion between substrate conformers is much higher than that of a chemical reaction. Namely, for any two different transition states with energies G_1^{TS} and G_2^{TS}, their contributions to the reaction (C_1 and C_2) are connected as following:

$$\frac{C1}{C2} = e^{\frac{G_2^{TS} - G_1^{TS}}{RT}}$$

where *R* is the gas constant and *T* is the temperature.

This equation was used to calculate contribution ratios between each TS and the lowest one, and then individual percentage contributions were calculated by considering the cumulative contribution to be 100%. Thermally-corrected (including zero-point correction, as well as vibrational, rotational, translational, enthalpy and entropy corrections at 408 K) energies of transition states were used to calculate contributions of each TS to the reaction.

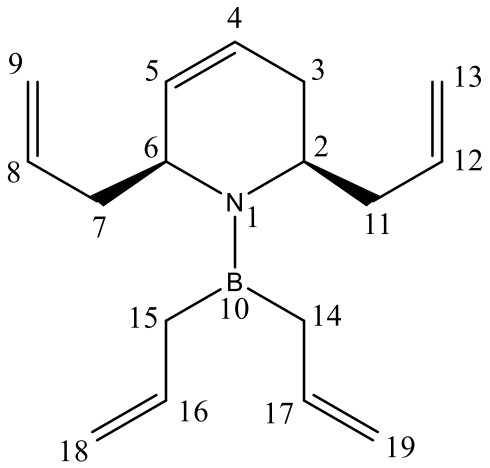
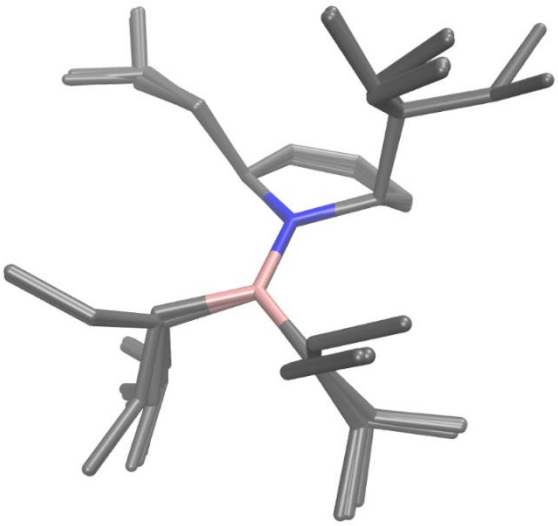
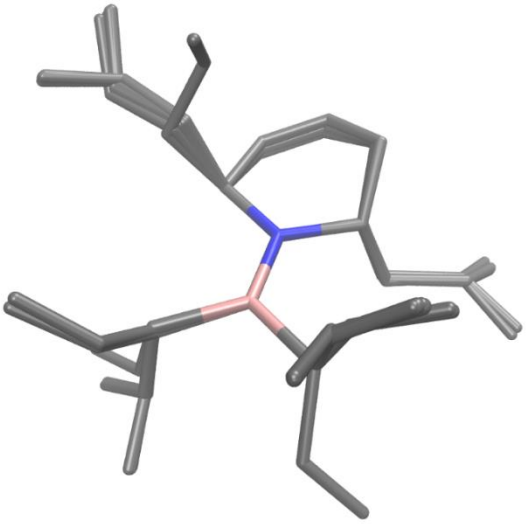


Figure S1. Numeration of atoms in ***cis*-3a**.

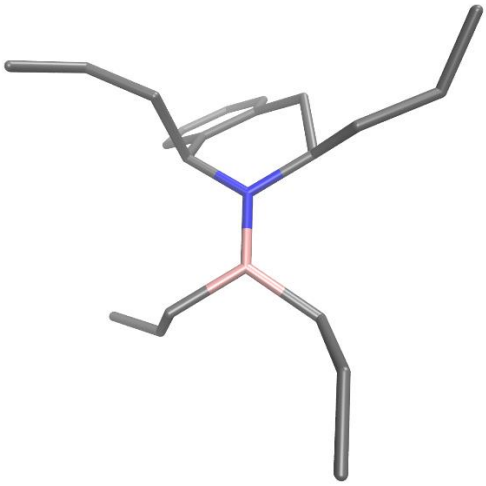
All conformers of ***cis*-3a**



All conformers of **3a**



Most stable conformer of ***cis*-3b**



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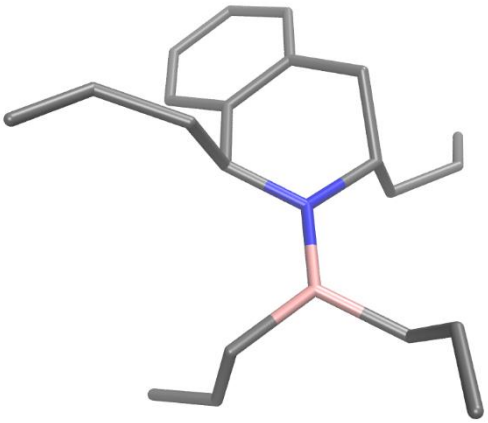
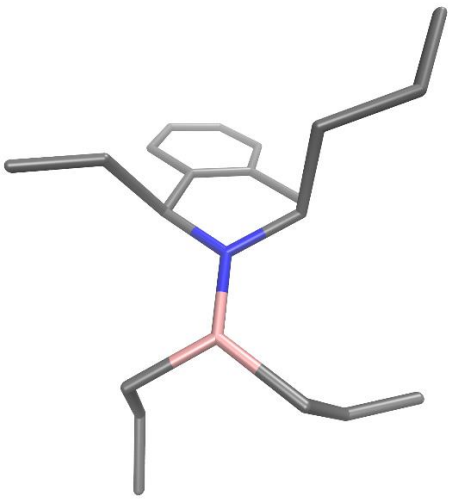


Most stable conformer of ***cis*-3c**



Most stable conformer of **3c**

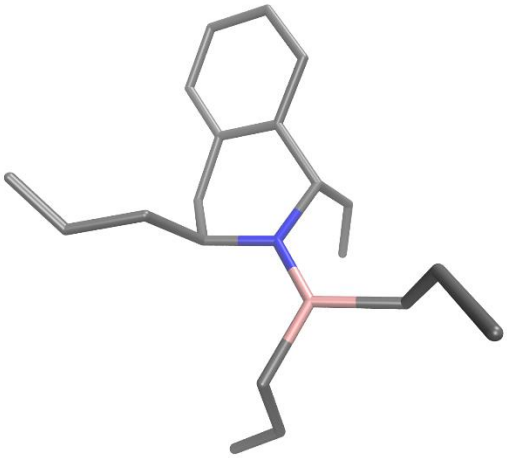
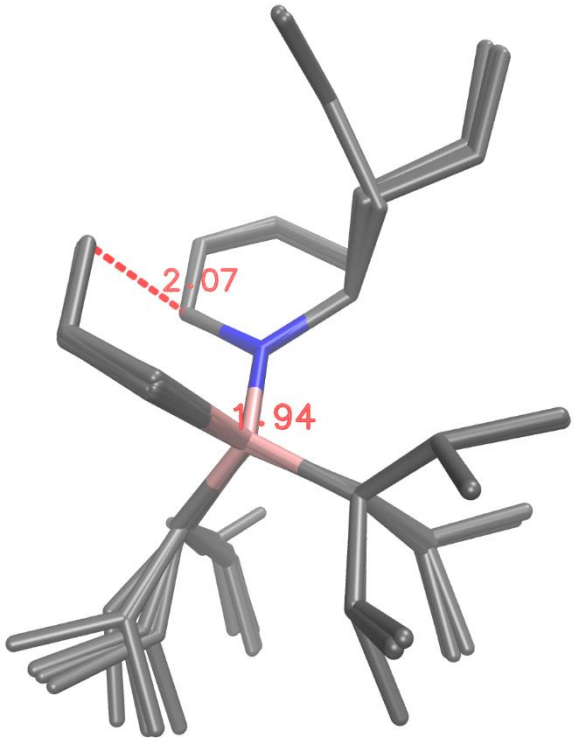
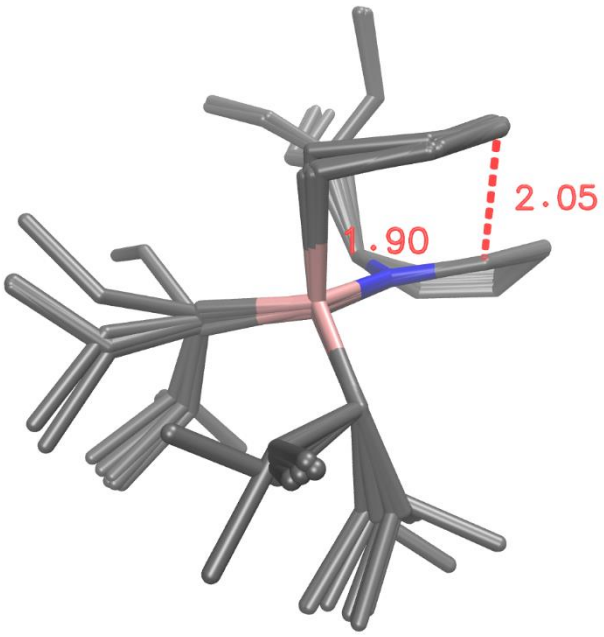


Figure S2. Top: superpositions of all located ***cis*-3a** and **3a** conformers; conformations are aligned by B1-N2-C3-C7 fragments, hydrogen atoms are omitted for clarity. Center and bottom: most stable conformers of ***cis*-3b**, ***cis*-3c**, **3b** and **3c**.

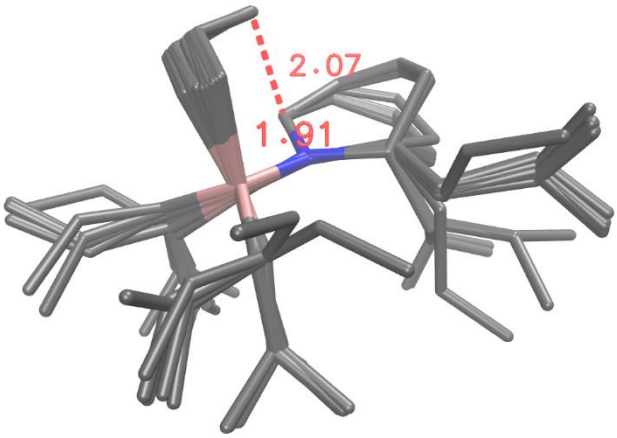
All located transition states *cis*-6



All located transition states *cis*-2



All located transition states *trans*-6



All located transition states *trans*-2

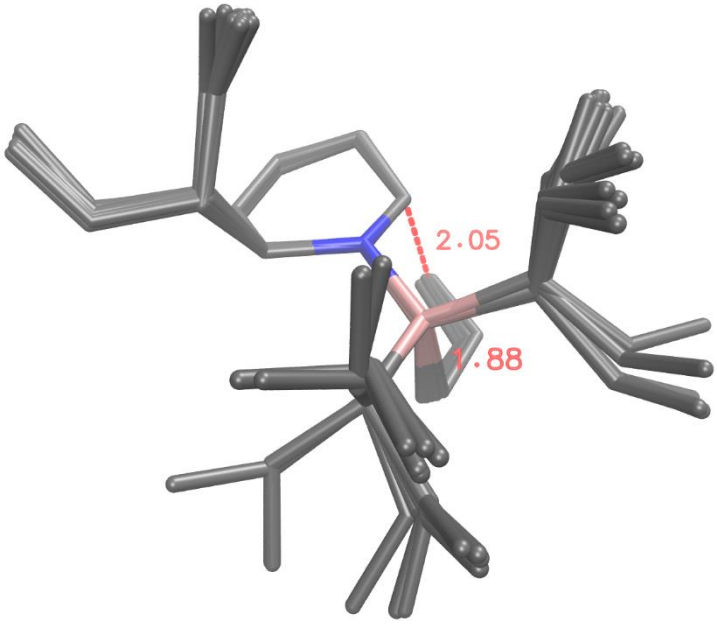


Figure S3. Superpositions of all located transition states conformations.
Conformations are aligned by B1-N2-C3-C7 fragments, hydrogen atoms are omitted for clarity.

Cartesian coordinates of all located stationary points:

3a:

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C       1.52659     -1.75788     -1.05822
C       0.90377     -2.75500     -0.11848
C      -1.97275     -1.27841     -0.80087
C       2.40873     -0.16040      0.73159
C       3.86059     -0.23898      0.34518
C       4.76608     -1.05846      0.89162
C      -3.10758     -2.17213     -0.38031
C      -3.49876     -3.27936     -1.02093
B      -0.35644      1.36823      0.03560
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C      -1.75638      1.81146      0.69175
C      -1.52071      2.28110      2.10591
C       0.23927      2.83099     -1.95437
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C      -4.40493     -1.69564     -0.90383
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H      5.64576    -1.39302     1.03488
H      4.20963    -2.10931     1.96119
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C     -0.94082    -2.16521     0.63934
C     -1.22757    -0.72463     0.28486
N     -0.00488     0.06792    -0.03813
C      1.25808    -0.66550    -0.31993
C      0.99955    -2.08877    -0.85061
C      0.06927    -2.83011     0.07226
C     -2.23264    -0.68619    -0.91261
C      2.16840    -0.69142     0.94071
C      3.57059    -1.16155     0.66154
C      4.19294    -2.16553     1.29089
C     -3.59762    -1.21752    -0.56730
C     -4.22124    -2.22058    -1.19626
B     -0.03199     1.47975    -0.00619
C      1.22437     2.37371    -0.47631
C     -1.31147     2.31421     0.50611
C     -1.08091     2.75789     1.93059
C      1.03192     2.79651    -1.91228
C     -1.82565     2.41223     2.99063
C      1.83616     2.48545    -2.93903
H     -1.63656    -2.65348     1.31766
H     -1.71254    -0.24897     1.14352
H      1.78398    -0.11380    -1.10449
H      1.95759    -2.60910    -0.94994
H      0.57388    -2.02870    -1.86314
H      0.24472    -3.88246     0.28708
H     -1.80791    -1.24695    -1.75354
H     -2.32726     0.35810    -1.23726
```

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H      1.70568    -1.31170     1.71730
H      2.21058     0.33232     1.33622
H      4.11019    -0.61460    -0.11544
H      5.21732    -2.44169     1.05119
H      3.70067    -2.74344     2.07196
H     -4.10659    -0.71935     0.26118
H     -5.21797    -2.54427    -0.90519
H     -3.75749    -2.75115    -2.02668
H      2.20070     1.88999    -0.36883
H      1.25189     3.27907     0.15050
H     -2.26818     1.78618     0.44594
H     -1.40636     3.21146    -0.12646
H     -0.21502     3.40178     2.09827
H      0.14101     3.39366    -2.11911
H     -1.58252     2.75791     3.99292
H     -2.70470     1.77667     2.89195
H      1.61620     2.81291    -3.95275
H      2.74258     1.89755    -2.80061
45
Bora-aza-Cope_3a E=-743.030259993 G=-742.724597 Imag-freq=0
C      1.36773    -1.96610    -0.84628
C      1.39622    -0.51300    -0.43220
N      0.06748     0.01251     0.00057
C     -1.00860    -0.96407     0.31744
C     -0.44661    -2.33020     0.75574
C      0.54394    -2.83746    -0.25786
C      2.45228    -0.32770     0.70650
C     -1.98119    -1.11678    -0.88681
C     -3.24717    -1.85602    -0.54663
C     -3.70424    -2.94266    -1.18054
C      3.86734    -0.56952     0.25498
C      4.71406    -1.45209     0.79780
B     -0.18231     1.40218     0.05055
C     -1.54861     2.00860     0.65003
C      0.86656     2.49469    -0.50108
C      0.50800     2.83873    -1.92655
C     -1.36255     2.33511     2.11113
C     -0.04363     3.98564    -2.34781
C     -2.05707     1.80894     3.13047
H      2.09790    -2.28114    -1.58802
H      1.72683     0.08153    -1.29023
H     -1.57537    -0.55613     1.15934
H     -1.27875    -3.03018     0.88177
H      0.02705    -2.23115     1.74341
H      0.55951    -3.89404    -0.51810
H      2.20014    -0.99244     1.54115
H      2.36732     0.70166     1.07809
H     -1.46424    -1.60951    -1.71869
H     -2.24097    -0.10614    -1.22914
H     -3.82966    -1.44669     0.28218
H     -4.63851    -3.42051    -0.89444
H     -3.16017    -3.38966    -2.01150
H      4.21247     0.04734    -0.57806
H      5.73250    -1.56424     0.43288
H      4.41892    -2.09076     1.62911
H     -2.42861     1.36738     0.53117
H     -1.76254     2.94191     0.10630
H      1.91035     2.16061    -0.47019
H      0.80367     3.40357     0.11316
H      0.69836     2.05657    -2.66496
H     -0.57324     3.05369     2.34346
H     -0.29612     4.14530    -3.39376
H     -0.25770     4.80384    -1.66137
H     -1.84802     2.08211     4.16245
H     -2.86062     1.09194     2.96721
45
Bora-aza-Cope_3a E=-743.030259993 G=-742.688358 Imag-freq=0
C      1.36773    -1.96610    -0.84628
C      1.39622    -0.51300    -0.43220
N      0.06748     0.01251     0.00057
C     -1.00860    -0.96407     0.31744
C     -0.44661    -2.33020     0.75574
C      0.54394    -2.83746    -0.25786
C      2.45228    -0.32770     0.70650
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C     -1.98119    -1.11678    -0.88681
C     -3.24717    -1.85602    -0.54663
C     -3.70424    -2.94266    -1.18054
C      3.86734    -0.56952     0.25498
C      4.71406    -1.45209     0.79780
B     -0.18231     1.40218     0.05055
C     -1.54861     2.00860     0.65003
C      0.86656     2.49469    -0.50108
C      0.50800     2.83873    -1.92655
C     -1.36255     2.33511     2.11113
C     -0.04363     3.98564    -2.34781
C     -2.05707     1.80894     3.13047
H      2.09790    -2.28114    -1.58802
H      1.72683     0.08153    -1.29023
H     -1.57537    -0.55613     1.15934
H     -1.27875    -3.03018     0.88177
H      0.02705    -2.23115     1.74341
H      0.55951    -3.89404    -0.51810
H      2.20014    -0.99244     1.54115
H      2.36732     0.70166     1.07809
H     -1.46424    -1.60951    -1.71869
H     -2.24097    -0.10614    -1.22914
H     -3.82966    -1.44669     0.28218
H     -4.63851    -3.42051    -0.89444
H     -3.16017    -3.38966    -2.01150
H      4.21247     0.04734    -0.57806
H      5.73250    -1.56424     0.43288
H      4.41892    -2.09076     1.62911
H     -2.42861     1.36738     0.53117
H     -1.76254     2.94191     0.10630
H      1.91035     2.16061    -0.47019
H      0.80367     3.40357     0.11316
H      0.69836     2.05657    -2.66496
H     -0.57324     3.05369     2.34346
H     -0.29612     4.14530    -3.39376
H     -0.25770     4.80384    -1.66137
H     -1.84802     2.08211     4.16245
H     -2.86062     1.09194     2.96721
45
Bora-aza-Cope_3a E=-743.030142099 G=-742.724071 Imag-freq=0
C      0.24790    -2.48551    -0.69998
C      0.95126    -1.20089    -0.32521
N      0.01537    -0.09036     0.02240
C     -1.39680    -0.43242     0.34320
C     -1.54583    -1.88013     0.85065
C     -0.89879    -2.83908    -0.11284
C      1.92892    -1.47237     0.86736
C     -2.31516    -0.17046    -0.88418
C     -3.78352    -0.22421    -0.55817
C     -4.68669    -1.00070    -1.16862
C      3.02495    -2.45171     0.54033
C      4.33118    -2.15847     0.52962
B      0.44866     1.25439     0.00806
C     -0.47682     2.46243     0.53435
C      1.89715     1.69395    -0.54581
C      1.76645     2.07619    -2.00022
C     -0.16726     2.74018     1.98452
C      1.80918     3.32071    -2.49684
C     -1.03347     2.65923     3.00500
H      0.74684    -3.13496    -1.41574
H      1.55524    -0.87584    -1.17759
H     -1.71618     0.23291     1.15070
H     -2.61002    -2.10285     0.97701
H     -1.09114    -1.96666     1.84815
H     -1.38396    -3.78538    -0.34384
H      1.33044    -1.85262     1.70636
H      2.36853    -0.52272     1.19008
H     -2.07483    -0.88137    -1.68346
H     -2.07429     0.83034    -1.26663
H     -4.11858     0.44377     0.23904
H     -5.73888    -0.97669    -0.89406
H     -4.40526    -1.68494    -1.96796
H      2.71314    -3.46871     0.29860
H      5.08172    -2.90756     0.28768
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H      4.69594    -1.16020     0.76784
H     -1.55414     2.30458     0.41670
H     -0.22208     3.35564    -0.05698
H      2.66055     0.91297    -0.45125
H      2.25630     2.56330     0.02205
H      1.59296     1.25001    -2.69347
H      0.86668     3.01255     2.20838
H      1.67969     3.51447    -3.55934
H      1.97947     4.18619    -1.85773
H     -0.72534     2.85596     4.02950
H     -2.07953     2.39800     2.85008
45
Bora-aza-Cope_3a E=-743.030142099 G=-742.687944 Imag-freq=0
C      0.24790    -2.48551    -0.69998
C      0.95126    -1.20089    -0.32521
N      0.01537    -0.09036     0.02240
C     -1.39680    -0.43242     0.34320
C     -1.54583    -1.88013     0.85065
C     -0.89879    -2.83908    -0.11284
C      1.92892    -1.47237     0.86736
C     -2.31516    -0.17046    -0.88418
C     -3.78352    -0.22421    -0.55817
C     -4.68669    -1.00070    -1.16862
C      3.02495    -2.45171     0.54033
C      4.33118    -2.15847     0.52962
B      0.44866     1.25439     0.00806
C     -0.47682     2.46243     0.53435
C      1.89715     1.69395    -0.54581
C      1.76645     2.07619    -2.00022
C     -0.16726     2.74018     1.98452
C      1.80918     3.32071    -2.49684
C     -1.03347     2.65923     3.00500
H      0.74684    -3.13496    -1.41574
H      1.55524    -0.87584    -1.17759
H     -1.71618     0.23291     1.15070
H     -2.61002    -2.10285     0.97701
H     -1.09114    -1.96666     1.84815
H     -1.38396    -3.78538    -0.34384
H      1.33044    -1.85262     1.70636
H      2.36853    -0.52272     1.19008
H     -2.07483    -0.88137    -1.68346
H     -2.07429     0.83034    -1.26663
H     -4.11858     0.44377     0.23904
H     -5.73888    -0.97669    -0.89406
H     -4.40526    -1.68494    -1.96796
H      2.71314    -3.46871     0.29860
H      5.08172    -2.90756     0.28768
H      4.69594    -1.16020     0.76784
H     -1.55414     2.30458     0.41670
H     -0.22208     3.35564    -0.05698
H      2.66055     0.91297    -0.45125
H      2.25630     2.56330     0.02205
H      1.59296     1.25001    -2.69347
H      0.86668     3.01255     2.20838
H      1.67969     3.51447    -3.55934
H      1.97947     4.18619    -1.85773
H     -0.72534     2.85596     4.02950
H     -2.07953     2.39800     2.85008
45
Bora-aza-Cope_3a E=-743.069375428 G=-742.758850 Imag-freq=0
C     -0.19679    -2.40771     0.55355
C     -0.88552    -1.08626     0.30606
N      0.04649     0.01770    -0.07039
C      1.43529    -0.33830    -0.46798
C      1.52659    -1.75788    -1.05822
C      0.90377    -2.75500    -0.11848
C     -1.97275    -1.27841    -0.80087
C      2.40873    -0.16040     0.73159
C      3.86059    -0.23898     0.34518
C      4.76608    -1.05846     0.89162
C     -3.10758    -2.17213    -0.38031
C     -3.49876    -3.27936    -1.02093
B     -0.35644     1.36823     0.03560
C      0.56224     2.57824    -0.50264
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C     -1.75638     1.81146     0.69175
C     -1.52071     2.28110     2.10591
C      0.23927     2.83099    -1.95437
C     -2.03086     1.72384     3.21325
C     -0.44383     3.87763    -2.43833
H     -0.67945    -3.09064     1.24735
H     -1.39693    -0.78970     1.22721
H      1.74132     0.36074    -1.25122
H      2.57737    -1.99509    -1.24755
H      1.02216    -1.77983    -2.03431
H      1.36711    -3.72849     0.02283
H     -1.49525    -1.67085    -1.70544
H     -2.37398    -0.28865    -1.05056
H      2.17896    -0.90023     1.50592
H      2.21265     0.82706     1.16827
H      4.18209     0.44836    -0.44008
H      5.80579    -1.04925     0.57575
H      4.49707    -1.76281     1.67640
H     -3.64863    -1.86460     0.51662
H     -4.34074    -3.87119    -0.67233
H     -2.99033    -3.62722    -1.91790
H      1.63591     2.38292    -0.40124
H      0.34735     3.48649     0.07376
H     -2.53271     1.04163     0.69419
H     -2.14381     2.65510     0.10075
H     -0.85664     3.13924     2.22275
H      0.57414     2.06604    -2.65735
H     -1.79561     2.10950     4.20165
H     -2.70247     0.86879     3.16616
H     -0.66041     3.97248    -3.49901
H     -0.80431     4.67293    -1.78871
45
Bora-aza-Cope_3a E=-743.030368203 G=-742.724624 Imag-freq=0
C     -0.21255    -2.40652     0.55118
C     -0.89284    -1.08022     0.30515
N      0.04609     0.01817    -0.07010
C      1.43302    -0.34555    -0.46711
C      1.51688    -1.76550    -1.05846
C      0.88638    -2.76000    -0.12059
C     -1.98082    -1.26471    -0.80271
C      2.40700    -0.17386     0.73331
C      3.85904    -0.25794     0.34649
C      4.76024    -1.08615     0.88796
C     -3.12261    -2.15028    -0.38174
C     -3.51825    -3.25840    -1.01904
B     -0.34880     1.37092     0.03682
C      0.57647     2.57718    -0.50166
C     -1.74605     1.82359     0.69451
C     -1.50496     2.28739     2.11035
C      0.25806     2.82708    -1.95551
C     -2.01470     1.72800     3.21734
C     -0.42275     3.87372    -2.44393
H     -0.70137    -3.08735     1.24409
H     -1.40216    -0.78014     1.22682
H      1.74264     0.35274    -1.25024
H      2.56748    -2.00900    -1.24644
H      1.01436    -1.78305    -2.03673
H      1.34446    -3.73719     0.01939
H     -1.50497    -1.66178    -1.70721
H     -2.37440    -0.27154    -1.05502
H      2.17374    -0.91492     1.50665
H      2.21450     0.81391     1.17324
H      4.18382     0.43327    -0.43507
H      5.80121    -1.08200     0.57263
H      4.48870    -1.79487     1.66920
H     -3.66449    -1.83491     0.51287
H     -4.36505    -3.84559    -0.67114
H     -3.00976    -3.61440    -1.91389
H      1.65084     2.38098    -0.39675
H      0.36301     3.48913     0.07164
H     -2.53007     1.05998     0.69608
H     -2.12925     2.67259     0.10637
H     -0.83646     3.14291     2.22782
H      0.59408     2.05883    -2.65545
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H     -1.77597     2.10833     4.20809
H     -2.69068     0.87520     3.17043
H     -0.63740     3.96775    -3.50613
H     -0.78484     4.67242    -1.79781
45
Bora-aza-Cope_3a E=-743.030368203 G=-742.688427 Imag-freq=0
C     -0.21255    -2.40652     0.55118
C     -0.89284    -1.08022     0.30515
N      0.04609     0.01817    -0.07010
C      1.43302    -0.34555    -0.46711
C      1.51688    -1.76550    -1.05846
C      0.88638    -2.76000    -0.12059
C     -1.98082    -1.26471    -0.80271
C      2.40700    -0.17386     0.73331
C      3.85904    -0.25794     0.34649
C      4.76024    -1.08615     0.88796
C     -3.12261    -2.15028    -0.38174
C     -3.51825    -3.25840    -1.01904
B     -0.34880     1.37092     0.03682
C      0.57647     2.57718    -0.50166
C     -1.74605     1.82359     0.69451
C     -1.50496     2.28739     2.11035
C      0.25806     2.82708    -1.95551
C     -2.01470     1.72800     3.21734
C     -0.42275     3.87372    -2.44393
H     -0.70137    -3.08735     1.24409
H     -1.40216    -0.78014     1.22682
H      1.74264     0.35274    -1.25024
H      2.56748    -2.00900    -1.24644
H      1.01436    -1.78305    -2.03673
H      1.34446    -3.73719     0.01939
H     -1.50497    -1.66178    -1.70721
H     -2.37440    -0.27154    -1.05502
H      2.17374    -0.91492     1.50665
H      2.21450     0.81391     1.17324
H      4.18382     0.43327    -0.43507
H      5.80121    -1.08200     0.57263
H      4.48870    -1.79487     1.66920
H     -3.66449    -1.83491     0.51287
H     -4.36505    -3.84559    -0.67114
H     -3.00976    -3.61440    -1.91389
H      1.65084     2.38098    -0.39675
H      0.36301     3.48913     0.07164
H     -2.53007     1.05998     0.69608
H     -2.12925     2.67259     0.10637
H     -0.83646     3.14291     2.22782
H      0.59408     2.05883    -2.65545
H     -1.77597     2.10833     4.20809
H     -2.69068     0.87520     3.17043
H     -0.63740     3.96775    -3.50613
H     -0.78484     4.67242    -1.79781
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3b/cis-3b:

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51
3b  E=-896.739100717 G=-896.386662 Imag-freq=0
C      4.43602    -0.35127     0.17603
C      3.85662    -1.39439     0.90522
C      2.47399    -1.59848     0.84925
C      1.66515    -0.77167     0.06042
C      2.24537     0.28617    -0.65840
C      3.62768     0.49257    -0.59271
C      0.17714    -1.02562    -0.08820
N     -0.63115     0.22751    -0.13386
C      0.05958     1.48339    -0.53380
C      1.30114     1.19714    -1.40036
C     -0.11249    -1.89290    -1.35976
C      0.41977     2.33381     0.71562
C      0.88070     3.72644     0.38035
C      2.02888     4.28149     0.78434
C      0.47062    -3.27929    -1.31025
C     -0.24926    -4.40751    -1.31170
B     -2.00262     0.21640     0.20565
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C     -2.94131     1.51129     0.01365
C     -2.73843    -1.08450     0.79816
C     -3.57425     1.46407    -1.35509
C     -2.82995    -0.97895     2.30008
C     -2.29142    -1.83370     3.18107
C     -4.85796     1.18567    -1.62082
H      5.50873    -0.18531     0.21799
H      4.47553    -2.04305     1.51841
H      2.02341    -2.40619     1.42055
H      4.07121     1.32221    -1.13786
H     -0.15215    -1.59978     0.78089
H     -0.63697     2.06314    -1.14545
H      0.98060     0.74726    -2.34840
H      1.79122     2.14257    -1.64983
H      0.28148    -1.36162    -2.23518
H     -1.19743    -1.95708    -1.48765
H      1.17757     1.81424     1.31232
H     -0.48163     2.39872     1.33768
H      0.19913     4.31821    -0.23401
H      2.29106     5.30243     0.52029
H      2.74235     3.73272     1.39572
H      1.55727    -3.35117    -1.27577
H      0.22595    -5.38429    -1.28171
H     -1.33679    -4.39163    -1.34838
H     -2.40027     2.45769     0.12618
H     -3.73211     1.50199     0.77424
H     -3.75813    -1.09783     0.38447
H     -2.27626    -2.03897     0.53052
H     -2.90356     1.64803    -2.19646
H     -3.36986    -0.11325     2.68791
H     -2.38357    -1.67663     4.25243
H     -1.74476    -2.71770     2.85844
H     -5.23002     1.14462    -2.64105
H     -5.57633     0.99374    -0.82615
51
Cis-3b E=-896.738168174 G=-896.385967 Imag-freq=0
C     -3.97595     0.65830    -2.00041
C     -3.96635    -0.62191    -1.43750
C     -2.91922    -1.00187    -0.59144
C     -1.88857    -0.10375    -0.29066
C     -1.90119     1.18305    -0.85044
C     -2.94168     1.55414    -1.71033
C     -0.71680    -0.48426     0.59677
N      0.54732    -0.00536    -0.01595
C      0.60351     1.43670    -0.39209
C     -0.78763     2.11685    -0.45802
C     -0.85870    -0.02406     2.07908
C      1.54739     2.23303     0.54485
C      1.81085     3.63702     0.07033
C      1.60895     4.74789     0.78754
C     -2.03013    -0.64712     2.78966
C     -1.93424    -1.47524     3.83627
B      1.60619    -0.89901    -0.30114
C      1.56314    -2.44819     0.13661
C      2.91517    -0.45838    -1.13129
C      0.97062    -3.32627    -0.93621
C     -0.07928    -4.14754    -0.79754
C      4.18716    -0.50237    -0.32310
C      5.18243    -1.38784    -0.46458
H     -4.78045     0.95590    -2.66696
H     -4.76223    -1.32536    -1.66477
H     -2.89994    -2.00372    -0.17010
H     -2.94378     2.54793    -2.15180
H     -0.66696    -1.57160     0.61639
H      1.02066     1.48007    -1.40266
H     -1.02081     2.55622     0.52133
H     -0.72794     2.95975    -1.15203
H      0.07125    -0.28679     2.59596
H     -0.95426     1.06718     2.12033
H      2.50064     1.69512     0.60048
H      1.13150     2.24835     1.55917
H      2.21074     3.72939    -0.94130
H      1.83768     5.73194     0.38756
H      1.21255     4.70848     1.80022
```

```
H     -3.01916     -0.39201      2.40937
H     -2.81677     -1.89324      4.31284
H     -0.96968     -1.75838      4.25319
H      1.04428     -2.62337      1.08611
H      2.60765     -2.75627      0.29146
H      2.81646      0.53730     -1.57916
H      3.01120     -1.16903     -1.96598
H      1.45067     -3.26916     -1.91508
H     -0.45029     -4.73912     -1.63026
H     -0.59981     -4.25535      0.15224
H      4.28678      0.25644      0.45525
H      6.06241     -1.35859      0.17240
H      5.14855     -2.16877     -1.22195
```

3c/cis-3c:

```
48
3c  E=-857.421884813 G=-857.093997 Imag-freq=0
C     -4.50935     -0.66673     -0.15260
C     -3.94636     -1.86656     -0.59949
C     -2.57165     -2.08419     -0.46049
C     -1.76002     -1.10966      0.13010
C     -2.32125      0.09728      0.57386
C     -3.69515      0.31440      0.42337
C     -0.27676     -1.35060      0.37779
N      0.56353     -0.14826      0.15262
C     -0.08976      1.18387      0.27661
C     -1.36433      1.11201      1.14119
C     -0.12324     -1.94637      1.77491
B      1.94012     -0.27527     -0.14203
C      2.91595      0.99603     -0.26262
C      2.62919     -1.70986     -0.37891
C      2.57989     -2.06591     -1.84368
C      3.69955      1.17039      1.01451
C      3.66617      2.24410      1.81624
C      3.62005     -2.07151     -2.68888
C      0.60227     -1.46144      2.78541
C     -0.38431      1.78628     -1.12446
C     -0.77555      3.23864     -1.07911
C     -1.88303      3.76190     -1.61702
H     -5.57563     -0.49053     -0.26201
H     -4.57172     -2.62633     -1.05924
H     -2.13155     -3.01461     -0.81153
H     -4.12846      1.25516      0.75407
H      0.04145     -2.12211     -0.33076
H      0.61459      1.84623      0.78813
H     -1.08308      0.84072      2.16635
H     -1.82571      2.10259      1.18447
H     -0.69276     -2.86480      1.91782
H      3.62199      0.78320     -1.07984
H      2.41737      1.93724     -0.51134
H      3.67793     -1.66327     -0.05937
H      2.15155     -2.50215      0.20910
H      1.59426     -2.31209     -2.24330
H      4.33186      0.33051      1.30765
H      4.24814      2.28478      2.73311
H      3.06031      3.11660      1.57937
H      3.49516     -2.31540     -3.74048
H      4.62850     -1.83623     -2.35399
H      0.63074     -1.97003      3.74468
H      1.18897     -0.55275      2.68749
H      0.52837      1.68344     -1.72433
H     -1.15979      1.19857     -1.62825
H     -0.07495      3.90387     -0.57045
H     -2.09289      4.82670     -1.56277
H     -2.61382      3.14250     -2.13312
48
Cis-3c  E=-857.421103305 G=-857.093588 Imag-freq=0
C     -3.89358     -1.16037     -1.82507
C     -3.56668     -2.26883     -1.03488
C     -2.40388     -2.24955     -0.26554
C     -1.54462     -1.13806     -0.27604
C     -1.86754     -0.03000     -1.07421
```

```
C     -3.04705    -0.05265    -1.83647
C     -0.26220    -1.19382     0.56289
N      0.59981     0.01087     0.41346
C     -0.10650     1.28706     0.16304
C     -0.94364     1.16254    -1.11636
C     -0.56936    -1.48272     2.02400
B      2.01080    -0.06456     0.49091
C      2.93798     1.24799     0.34013
C      2.78080    -1.46225     0.69815
C      3.28874    -2.00153    -0.61572
C      3.14053     1.69415    -1.08701
C      2.85737     2.90522    -1.58593
C      4.57216    -2.08633    -0.99155
C     -0.92813     1.78500     1.38163
C     -1.34611     3.22500     1.24605
C     -0.28338    -2.63273     2.64176
C     -2.60341     3.67537     1.32061
H     -4.80081    -1.15978    -2.42249
H     -4.21489    -3.14021    -1.01559
H     -2.15748    -3.10761     0.35345
H     -3.29777     0.81406    -2.44367
H      0.30871    -2.04399     0.18073
H      0.66236     2.03462    -0.02421
H     -1.51926     2.08012    -1.27801
H     -0.25605     1.06813    -1.96718
H     -1.06275    -0.68804     2.57863
H      2.56315     2.08951     0.93732
H      3.92352     0.99144     0.75470
H      3.63467    -1.29199     1.36683
H      2.15133    -2.21913     1.17784
H      2.52395    -2.33040    -1.32222
H      3.55766     0.94349    -1.75953
H      3.03155     3.14214    -2.63219
H      2.44405     3.69822    -0.96525
H      4.85294    -2.47053    -1.96859
H      5.38115    -1.77513    -0.33339
H     -0.28942     1.68153     2.26918
H     -1.81456     1.16201     1.54116
H     -0.53848     3.94130     1.08458
H     -0.53445    -2.79067     3.68686
H      0.20585    -3.45664     2.12642
H     -2.83471     4.73311     1.22953
H     -3.44182     3.00013     1.47946
```

4a:

```
45
bora-aza-Cope_4a E=-743.048582784 G=-742.739767 Imag-freq=0
C      1.18870    -2.65303    -0.07455
C      0.08724    -1.77380     0.28546
N      0.04433    -0.50430     0.01879
C      1.27993     0.10172    -0.56335
C      1.96316    -0.85173    -1.55445
C      2.08185    -2.23761    -0.99150
C     -2.25684     0.00808    -1.13336
C      2.22239     0.53251     0.59396
C      3.32522     1.44569     0.13052
C      4.63295     1.19427     0.25258
C     -2.74511    -1.39580    -1.25306
C     -2.29853    -2.32595    -2.11452
B     -1.33160     0.35441     0.21003
C     -1.04201     1.99326     0.30302
C     -2.08925    -0.13741     1.60107
C     -1.33038     0.11246     2.86699
C     -0.99208     2.79981    -0.96319
C     -0.92053    -0.81264     3.74987
C     -1.88621     3.72382    -1.34705
H      1.19696    -3.65528     0.33914
H     -0.77548    -2.20392     0.77928
H      0.96471     0.99412    -1.10059
H      2.94860    -0.44812    -1.80766
H      1.40248    -0.90113    -2.50034
H      2.85720    -2.90226    -1.36233
```

H	-1.70219	0.28842	-2.03955
H	-3.11826	0.68988	-1.06945
H	3.00719	2.38305	-0.32840
H	5.38161	1.90443	-0.08727
H	4.99687	0.27274	0.70239
H	-3.51666	-1.69880	-0.54206
H	-2.68614	-3.34160	-2.11149
H	-1.53360	-2.09509	-2.85428
H	-0.12205	2.18471	0.87488
H	-1.85396	2.40529	0.91915
H	-2.40382	-1.18975	1.57142
H	-3.02160	0.44890	1.62345
H	-1.06638	1.15301	3.06815
H	-0.15698	2.61384	-1.64243
H	-0.34345	-0.54499	4.63156
H	-1.15199	-1.86863	3.61851
H	-1.78917	4.25598	-2.29007
H	-2.74760	3.97286	-0.72897
H	1.61561	1.05227	1.34377
H	2.64283	-0.35377	1.08087

4’a:

```
45
bora-aza-Cope_4a' E=-743.040871498 G=-742.731951 Imag-freq=0
C      2.67642    -1.11484    -0.68458
C      1.73257     0.01902    -0.36088
N      0.54918    -0.44927     0.42413
C      0.72620    -1.41287     1.25727
C      1.99703    -2.19079     1.41427
C      2.83311    -2.13169     0.16396
C      2.46726     1.14003     0.43572
C     -1.99170    -0.35520     1.23745
C     -3.38444     0.19521     1.16406
C     -4.50330    -0.50482     0.91946
C      3.48731     1.86386    -0.40141
C      4.79106     1.94853    -0.11801
B     -0.96118     0.15882     0.05433
C     -0.82764     1.80565    -0.03853
C     -1.33106    -0.49240    -1.43064
C     -1.17225    -1.97364    -1.57855
C     -1.96292     2.54275    -0.69053
C     -2.15578    -2.88397    -1.65606
C     -2.64931     3.57300    -0.17450
H      3.24807    -1.04039    -1.60448
H      1.33913     0.44839    -1.28395
H      1.73408    -3.22078     1.67979
H      2.54931    -1.80369     2.28577
H      3.53131    -2.94068    -0.02898
H      2.94503     0.69760     1.31633
H      1.71892     1.85557     0.79195
H     -1.56756    -0.05590     2.21144
H     -2.06455    -1.45242     1.24334
H     -3.48277     1.26876     1.31855
H     -5.47750    -0.02397     0.87455
H     -4.47900    -1.57990     0.74929
H      3.10527     2.36074    -1.29442
H      5.47438     2.50452    -0.75374
H      5.21594     1.46913     0.76136
H      0.05878     2.04423    -0.64577
H     -0.64502     2.24189     0.95557
H     -0.72576     0.00521    -2.20531
H     -2.37513    -0.21836    -1.63282
H     -0.14521    -2.34441    -1.60849
H     -2.22888     2.21243    -1.69661
H     -1.94349    -3.94698    -1.74011
H     -3.20450    -2.59314    -1.63536
H     -3.45132     4.05744    -0.72593
H     -2.43788     3.95714     0.82238
H     -0.12539    -1.71869     1.85404
```

Cis-3a:

```
45
Bora-aza-Cope_cis-3a E=-743.035796974 G=-742.729854 Imag-freq=0
C     -0.45678    -2.03997     1.21890
C     -0.89381    -1.03337     0.18323
N     -0.12619     0.23426     0.26451
C      1.29066     0.10738     0.67743
C      1.38837    -0.59377     2.04469
C      0.54796    -1.84168     2.07860
C     -0.91424    -1.64280    -1.25380
C      2.17413    -0.57869    -0.40101
C      3.64375    -0.33016    -0.18678
C      4.57926    -1.27778    -0.05290
C     -1.97495    -2.69669    -1.42896
C     -1.75866    -3.95153    -1.84058
B     -0.74084     1.47766     0.00108
C      0.03042     2.88502     0.14170
C     -2.28355     1.58560    -0.45411
C     -3.16851     1.87824     0.73225
C      0.62632     3.31895    -1.17444
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C     -4.18142     1.11553     1.16822
C      1.92260     3.56419    -1.41176
H     -1.03534    -2.96118     1.24781
H     -1.93270    -0.78134     0.42401
H      1.67270     1.12194     0.78955
H      1.06841     0.09998     2.83649
H      2.43712    -0.83579     2.25815
H      0.78390    -2.60039     2.82357
H      0.06677    -2.05452    -1.51102
H     -1.11147    -0.81680    -1.95080
H      1.88202    -0.16564    -1.37640
H      1.98458    -1.65735    -0.43117
H      3.94787     0.71843    -0.15228
H      5.62889    -1.02758     0.08373
H      4.32837    -2.33732    -0.07950
H     -2.99785    -2.38469    -1.20626
H     -2.57449    -4.66047    -1.96182
H     -0.75795    -4.31232    -2.07414
H      0.80408     2.90149     0.91852
H     -0.72128     3.63415     0.43857
H     -2.66540     0.70833    -0.98798
H     -2.35492     2.43296    -1.15540
H     -2.93684     2.79025     1.28706
H     -0.07820     3.42606    -2.00256
H     -4.75942     1.38785     2.04854
H     -4.46988     0.19690     0.65894
H      2.27446     3.85898    -2.39792
H      2.67485     3.47911    -0.62867
45
Bora-aza-Cope_cis-3a E=-743.035796974 G=-742.693648 Imag-freq=0
C     -0.45678    -2.03997     1.21890
C     -0.89381    -1.03337     0.18323
N     -0.12619     0.23426     0.26451
C      1.29066     0.10738     0.67743
C      1.38837    -0.59377     2.04469
C      0.54796    -1.84168     2.07860
C     -0.91424    -1.64280    -1.25380
C      2.17413    -0.57869    -0.40101
C      3.64375    -0.33016    -0.18678
C      4.57926    -1.27778    -0.05290
C     -1.97495    -2.69669    -1.42896
C     -1.75866    -3.95153    -1.84058
B     -0.74084     1.47766     0.00108
C      0.03042     2.88502     0.14170
C     -2.28355     1.58560    -0.45411
C     -3.16851     1.87824     0.73225
C      0.62632     3.31895    -1.17444
C     -4.18142     1.11553     1.16822
C      1.92260     3.56419    -1.41176
H     -1.03534    -2.96118     1.24781
H     -1.93270    -0.78134     0.42401
H      1.67270     1.12194     0.78955
H      1.06841     0.09998     2.83649
H      2.43712    -0.83579     2.25815
H      0.78390    -2.60039     2.82357
H      0.06677    -2.05452    -1.51102
H     -1.11147    -0.81680    -1.95080
H      1.88202    -0.16564    -1.37640
H      1.98458    -1.65735    -0.43117
H      3.94787     0.71843    -0.15228
H      5.62889    -1.02758     0.08373
H      4.32837    -2.33732    -0.07950
H     -2.99785    -2.38469    -1.20626
H     -2.57449    -4.66047    -1.96182
H     -0.75795    -4.31232    -2.07414
H      0.80408     2.90149     0.91852
H     -0.72128     3.63415     0.43857
H     -2.66540     0.70833    -0.98798
H     -2.35492     2.43296    -1.15540
H     -2.93684     2.79025     1.28706
H     -0.07820     3.42606    -2.00256
H     -4.75942     1.38785     2.04854
H     -4.46988     0.19690     0.65894
H      2.27446     3.85898    -2.39792
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H      2.67485     3.47911    -0.62867
45
Bora-aza-Cope_cis-3a E=-743.075113167 G=-742.765029 Imag-freq=0
C     -1.08622     1.87134     1.29383
C     -0.09182     1.45779     0.23769
N      0.20683     0.00417     0.27483
C     -0.91718    -0.87640     0.66975
C     -1.46000    -0.46606     2.05043
C     -1.68639     1.01867     2.13040
C     -0.50326     1.96013    -1.18208
C     -2.03417    -0.95097    -0.40764
C     -2.94554    -2.13271    -0.21124
C     -4.27454    -2.07226    -0.07021
C     -0.44042     3.45795    -1.31426
C     -1.45685     4.24541    -1.68327
B      1.49657    -0.49074    -0.02095
C      1.86970    -2.05433     0.04372
C      2.70842     0.48444    -0.44232
C      3.54116     0.84042     0.76341
C      1.68421    -2.72387    -1.29423
C      4.77372     0.38767     1.03155
C      0.88853    -3.77133    -1.55021
H     -1.28370     2.93863     1.35725
H      0.84149     1.97677     0.48196
H     -0.50645    -1.88177     0.75492
H     -0.75315    -0.78192     2.83091
H     -2.39430    -1.00326     2.25117
H     -2.36765     1.39479     2.89119
H     -1.50504     1.60466    -1.43866
H      0.19564     1.50851    -1.89804
H     -1.53976    -1.04209    -1.38366
H     -2.62662    -0.03045    -0.42298
H     -2.45921    -3.10979    -0.19459
H     -4.87436    -2.96974     0.05423
H     -4.80638    -1.12284    -0.07878
H      0.52602     3.91559    -1.09433
H     -1.33830     5.32171    -1.77368
H     -2.43994     3.83797    -1.91051
H      1.32525    -2.61377     0.81263
H      2.93533    -2.11033     0.31276
H      2.36436     1.40448    -0.92939
H      3.34158    -0.04113    -1.16923
H      3.07096     1.50784     1.48813
H      2.25066    -2.29475    -2.12317
H      5.29736     0.67195     1.94035
H      5.29738    -0.27883     0.34891
H      0.80152    -4.18630    -2.55083
H      0.30064    -4.24690    -0.76753
45
Bora-aza-Cope_cis-3a E=-743.075113167 G=-742.765029 Imag-freq=0
C     -1.08622     1.87134     1.29383
C     -0.09182     1.45779     0.23769
N      0.20683     0.00417     0.27483
C     -0.91718    -0.87640     0.66975
C     -1.46000    -0.46606     2.05043
C     -1.68639     1.01867     2.13040
C     -0.50326     1.96013    -1.18208
C     -2.03417    -0.95097    -0.40764
C     -2.94554    -2.13271    -0.21124
C     -4.27454    -2.07226    -0.07021
C     -0.44042     3.45795    -1.31426
C     -1.45685     4.24541    -1.68327
B      1.49657    -0.49074    -0.02095
C      1.86970    -2.05433     0.04372
C      2.70842     0.48444    -0.44232
C      3.54116     0.84042     0.76341
C      1.68421    -2.72387    -1.29423
C      4.77372     0.38767     1.03155
C      0.88853    -3.77133    -1.55021
H     -1.28370     2.93863     1.35725
H      0.84149     1.97677     0.48196
H     -0.50645    -1.88177     0.75492
H     -0.75315    -0.78192     2.83091
H     -2.39430    -1.00326     2.25117
```

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H     -2.36765     1.39479     2.89119
H     -1.50504     1.60466    -1.43866
H      0.19564     1.50851    -1.89804
H     -1.53976    -1.04209    -1.38366
H     -2.62662    -0.03045    -0.42298
H     -2.45921    -3.10979    -0.19459
H     -4.87436    -2.96974     0.05423
H     -4.80638    -1.12284    -0.07878
H      0.52602     3.91559    -1.09433
H     -1.33830     5.32171    -1.77368
H     -2.43994     3.83797    -1.91051
H      1.32525    -2.61377     0.81263
H      2.93533    -2.11033     0.31276
H      2.36436     1.40448    -0.92939
H      3.34158    -0.04113    -1.16923
H      3.07096     1.50784     1.48813
H      2.25066    -2.29475    -2.12317
H      5.29736     0.67195     1.94035
H      5.29738    -0.27883     0.34891
H      0.80152    -4.18630    -2.55083
H      0.30064    -4.24690    -0.76753
45
Bora-aza-Cope_cis-3a E=-743.035955637 G=-742.730697 Imag-freq=0
C     -1.07497     1.87810     1.29201
C     -0.08324     1.45785     0.23546
N      0.20616     0.00222     0.27296
C     -0.92346    -0.87111     0.66806
C     -1.46321    -0.45739     2.04924
C     -1.68031     1.02916     2.12898
C     -0.49287     1.96190    -1.18464
C     -2.04219    -0.93805    -0.40867
C     -2.95762    -2.11777    -0.21443
C     -4.28574    -2.05249    -0.06326
C     -0.41572     3.45948    -1.31859
C     -1.42706     4.25742    -1.68069
B      1.49303    -0.50027    -0.02236
C      1.86059    -2.06626     0.04331
C      2.71189     0.46772    -0.44434
C      3.54036     0.82673     0.76424
C      1.66932    -2.73626    -1.29437
C      4.76923     0.36837     1.04202
C      0.86875    -3.78112    -1.54801
H     -1.26489     2.94766     1.35484
H      0.85455     1.97002     0.47852
H     -0.51869    -1.87928     0.75279
H     -0.75736    -0.77853     2.82986
H     -2.40140    -0.98951     2.25064
H     -2.35998     1.40893     2.89065
H     -1.49934     1.61541    -1.43865
H      0.19998     1.50174    -1.90247
H     -1.54971    -1.02664    -1.38692
H     -2.63159    -0.01460    -0.41964
H     -2.47436    -3.09731    -0.20823
H     -4.89037    -2.94818     0.05976
H     -4.81535    -1.10073    -0.06119
H      0.55796     3.90683    -1.10588
H     -1.29947     5.33357    -1.77275
H     -2.41728     3.86123    -1.90117
H      1.31729    -2.62567     0.81463
H      2.92774    -2.12696     0.30986
H      2.37665     1.38773    -0.94024
H      3.34779    -0.06500    -1.16532
H      3.06876     1.50123     1.48257
H      2.23634    -2.30906    -2.12489
H      5.29111     0.65426     1.95256
H      5.29448    -0.30573     0.36662
H      0.77677    -4.19778    -2.54862
H      0.27961    -4.25539    -0.76415
45
Bora-aza-Cope_cis-3a E=-743.035955637 G=-742.694298 Imag-freq=0
C     -1.07497     1.87810     1.29201
C     -0.08324     1.45785     0.23546
N      0.20616     0.00222     0.27296
C     -0.92346    -0.87111     0.66806
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C      -1.46321     -0.45739      2.04924
C      -1.68031      1.02916      2.12898
C      -0.49287      1.96190     -1.18464
C      -2.04219     -0.93805     -0.40867
C      -2.95762     -2.11777     -0.21443
C      -4.28574     -2.05249     -0.06326
C      -0.41572      3.45948     -1.31859
C      -1.42706      4.25742     -1.68069
B       1.49303     -0.50027     -0.02236
C       1.86059     -2.06626      0.04331
C       2.71189      0.46772     -0.44434
C       3.54036      0.82673      0.76424
C       1.66932     -2.73626     -1.29437
C       4.76923      0.36837      1.04202
C       0.86875     -3.78112     -1.54801
H      -1.26489      2.94766      1.35484
H       0.85455      1.97002      0.47852
H      -0.51869     -1.87928      0.75279
H      -0.75736     -0.77853      2.82986
H      -2.40140     -0.98951      2.25064
H      -2.35998      1.40893      2.89065
H      -1.49934      1.61541     -1.43865
H       0.19998      1.50174     -1.90247
H      -1.54971     -1.02664     -1.38692
H      -2.63159     -0.01460     -0.41964
H      -2.47436     -3.09731     -0.20823
H      -4.89037     -2.94818      0.05976
H      -4.81535     -1.10073     -0.06119
H       0.55796      3.90683     -1.10588
H      -1.29947      5.33357     -1.77275
H      -2.41728      3.86123     -1.90117
H       1.31729     -2.62567      0.81463
H       2.92774     -2.12696      0.30986
H       2.37665      1.38773     -0.94024
H       3.34779     -0.06500     -1.16532
H       3.06876      1.50123      1.48257
H       2.23634     -2.30906     -2.12489
H       5.29111      0.65426      1.95256
H       5.29448     -0.30573      0.36662
H       0.77677     -4.19778     -2.54862
H       0.27961     -4.25539     -0.76415
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TS_cis-2:

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45
bora-aza-Cope_TS-cis-2-conf10 E=-743.015788144 G=-742.701014 Imag-freq=1
C       1.70161     -0.00062     -1.75148
C       1.08544      0.37767     -0.42629
N      -0.14910     -0.40648     -0.16453
C      -0.18876     -1.71209     -0.52107
C       0.78991     -2.29041     -1.53916
C       1.57494     -1.22758     -2.25785
C       2.14824      0.28187      0.71172
C       0.17046     -2.76016      1.23361
C      -0.86649     -2.19836      1.97855
C      -0.90598     -0.83696      2.36330
C       3.26139      1.28205      0.54848
C       4.56394      0.98493      0.48937
B      -1.25631      0.12363      0.73876
C      -2.78211     -0.30996      0.32071
C      -1.11998      1.68460      1.23532
C      -1.49726      2.74803      0.24372
C      -3.31406     -0.04999     -1.07222
C      -0.72235      3.76404     -0.16672
C      -2.66884      0.44394     -2.13750
H       2.28936      0.76044     -2.25689
H       0.76579      1.42072     -0.48155
H      -1.19382     -2.09853     -0.62772
H       0.21750     -2.89216     -2.25493
H       1.48772     -2.99293     -1.06537
H       2.04803     -1.50111     -3.19796
H       2.56207     -0.73092      0.75318
H       1.64599      0.47451      1.66613
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H      1.18506    -2.39514     1.36323
H      0.09526    -3.80186     0.93039
H     -1.80508     -2.75281     2.00307
H     -1.74482     -0.54044     2.99355
H      0.03433    -0.39149     2.68330
H      2.95538     2.32799     0.49073
H      5.31896     1.75990     0.39007
H      4.91734    -0.04288     0.54124
H     -3.46680     0.19397     1.02401
H     -2.97394     -1.37583     0.52022
H     -0.12687     1.91078     1.64590
H     -1.81744     1.76379     2.08406
H     -2.49919     2.66882     -0.17860
H     -4.36361     -0.32351     -1.21399
H     -1.07225     4.48861     -0.89785
H      0.28808     3.90302     0.21485
H     -3.17732     0.56867     -3.09074
H     -1.62520     0.73961     -2.09529
45
bora-aza-Cope_TS-cis-2-conf11 E=-743.021709797 G=-742.708055 Imag-freq=1
C      2.25512    -0.63730     -1.55350
C      1.28304     0.23482     -0.79508
N      0.23692    -0.58057     -0.12656
C      0.59543    -1.75675     0.44841
C      1.91638    -2.44025     0.10023
C      2.55238    -1.86885     -1.13819
C      2.04772     1.19041     0.17258
C      0.69957    -1.37734     2.46387
C     -0.58959     -0.86176     2.61134
C     -1.00582     0.36344     2.03563
C      2.90663     2.18788     -0.55734
C      4.22144     2.35296     -0.37744
B     -1.14708     -0.00413     0.19784
C     -2.37714     -1.08489     0.02630
C     -1.45109     1.44276     -0.51788
C     -2.77030     2.06438     -0.16839
C     -2.61487     -1.48918     -1.39982
C     -2.95226     3.22351     0.48186
C     -3.72776     -1.27828     -2.11849
H      2.73079    -0.20411     -2.42872
H      0.75666     0.86442     -1.51617
H     -0.22306     -2.45602     0.55444
H      1.72295    -3.51152     -0.02462
H      2.62990    -2.36973     0.93152
H      3.27474    -2.48608     -1.66677
H      2.66254     0.60571     0.86472
H      1.30741     1.73706     0.76745
H      1.54221    -0.69417     2.40379
H      0.93003    -2.34844     2.89608
H     -1.36738     -1.56098     2.92016
H     -2.01202     0.69826     2.28635
H     -0.28250     1.17790     2.05721
H      2.38811     2.82413     -1.27675
H      4.77928     3.10641     -0.92661
H      4.78176     1.74187     0.32721
H     -3.29839     -0.65745     0.44364
H     -2.18237     -1.99268     0.61478
H     -1.44222     1.26472     -1.60616
H     -0.65874     2.17388     -0.31317
H     -3.65824     1.50893     -0.47340
H     -1.77838     -1.98876     -1.89452
H     -3.94647     3.60067     0.70783
H     -2.11054     3.83074     0.81126
H     -3.80339     -1.58752     -3.15805
H     -4.59903     -0.78606     -1.68934
45
bora-aza-Cope_TS-cis-2-conf12 E=-743.018043869 G=-742.703392 Imag-freq=1
C      1.98268    -1.20693     -1.83751
C      1.02795    -0.13303     -1.37634
N      0.29936    -0.54033     -0.14767
C      0.92485    -1.30071     0.78719
C      2.25077    -1.99581     0.48775
C      2.54268    -2.06738     -0.98707
C      1.73692     1.26107     -1.35107
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C      1.31662    -0.04948     2.36368
C      0.02710     0.46028     2.53017
C     -0.61852     1.26484     1.55819
C      3.01708     1.38508    -0.56953
C      3.31947     2.40642     0.24006
B     -1.07083     0.05434     0.20463
C     -2.12383    -1.03332     0.85582
C     -1.74743     0.94978    -0.99608
C     -3.05368     1.60002    -0.64967
C     -2.56680    -2.08485    -0.11977
C     -3.29116     2.91917    -0.59396
C     -3.81835    -2.30690    -0.54870
H      2.21807    -1.22418    -2.89902
H      0.25412    -0.03419    -2.14171
H      0.25180    -1.91607     1.36923
H      2.21805    -2.99961     0.92549
H      3.08496    -1.48672     0.98823
H      3.24598    -2.82312    -1.32849
H      1.02747     2.02881    -1.03053
H      1.96436     1.47604    -2.40606
H      2.05373     0.54094     1.82916
H      1.71913    -0.71284     3.12651
H     -0.60203    -0.01396     3.28404
H     -1.58626     1.68052     1.83873
H      0.00724     1.98645     1.03395
H      3.75685     0.60062    -0.72620
H      4.28026     2.46503     0.74407
H      2.61794     3.21717     0.42666
H     -3.00249    -0.50280     1.24606
H     -1.67745    -1.53711     1.72463
H     -1.92979     0.25997    -1.83705
H     -1.06563     1.72361    -1.36851
H     -3.87994     0.92620    -0.41912
H     -1.77228    -2.71506    -0.52704
H     -4.26781     3.31186    -0.32232
H     -2.51378     3.64858    -0.81621
H     -4.04336    -3.08185    -1.27730
H     -4.65862    -1.71724    -0.18560
45
bora-aza-Cope_TS-cis-2-conf13 E=-743.018779658 G=-742.704119 Imag-freq=1
C      1.62245    -0.84910    -1.80043
C      1.06157     0.04255    -0.71496
N     -0.19880    -0.52797    -0.17494
C     -0.24477    -1.86313     0.06576
C      0.79818    -2.80098    -0.53993
C      1.50409    -2.17488    -1.71626
C      2.14082     0.31314     0.37798
C     -0.05087    -2.06490     2.09632
C     -1.09007    -1.20978     2.47095
C     -1.05996     0.18784     2.24092
C      3.32120     1.08143    -0.15077
C      4.59470     0.67632    -0.09534
B     -1.32089     0.34902     0.38010
C     -2.83470    -0.23882     0.08142
C     -1.27198     1.95321     0.02159
C     -0.24556     2.87149     0.61948
C     -3.21439    -0.19778    -1.36963
C      0.57536     3.69362    -0.05028
C     -4.19925     0.52819    -1.92000
H      2.15443    -0.37395    -2.61960
H      0.79506     1.00736    -1.14937
H     -1.24386    -2.27726     0.05083
H      0.29690    -3.72911    -0.83317
H      1.54731    -3.09572     0.20679
H      1.92693    -2.83540    -2.46912
H      2.47958    -0.63360     0.81134
H      1.67142     0.90031     1.17465
H      0.97286    -1.70480     2.14181
H     -0.16478    -3.13397     2.26116
H     -2.05967    -1.66673     2.66982
H     -1.89077     0.76223     2.65284
H     -0.09924     0.67567     2.39554
H      3.09135     2.04978    -0.59715
H      5.40299     1.29094    -0.48214
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H 4.87094 -0.28148 0.34106
H -3.55798 0.34907 0.66347
H -2.93817 -1.27412 0.43531
H -2.25675 2.32666 0.34513
H -1.26577 2.07275 -1.07214
H -0.19145 2.88566 1.70990
H -2.60485 -0.81385 -2.03538
H 1.28162 4.33953 0.46516
H 0.57103 3.74248 -1.13823
H -4.38992 0.51430 -2.99031
H -4.84406 1.16355 -1.31488
45
bora-aza-Cope_TS-cis-2-conf14 E=-743.017980858 G=-742.704014 Imag-freq=1
C 1.83702 0.19339 -1.83187
C 1.15160 0.57441 -0.54123
N 0.11585 -0.42470 -0.16961
C 0.38360 -1.73950 -0.36131
C 1.48886 -2.19746 -1.30937
C 2.00057 -1.08298 -2.18094
C 2.20666 0.83576 0.57798
C 0.92903 -2.46167 1.50168
C -0.22924 -2.06983 2.17299
C -0.58631 -0.71770 2.39437
C 3.06894 2.03538 0.28901
C 4.40458 2.02798 0.22367
B -1.09831 -0.05420 0.68351
C -2.47840 -0.85911 0.27867
C -1.31284 1.54292 0.99061
C -1.93200 2.38583 -0.09042
C -2.84348 -0.83217 -1.18043
C -3.03502 3.13772 0.03508
C -4.00668 -0.43116 -1.71263
H 2.22777 1.00210 -2.44267
H 0.61919 1.51392 -0.70167
H -0.50089 -2.36034 -0.41062
H 1.09198 -3.01392 -1.92360
H 2.33033 -2.63501 -0.75673
H 2.52306 -1.35662 -3.09432
H 2.83564 -0.05008 0.71205
H 1.67225 1.00850 1.51895
H 1.82962 -1.86099 1.58851
H 1.10123 -3.52081 1.32502
H -1.01842 -2.81702 2.26201
H -1.48575 -0.55268 2.98811
H 0.22103 -0.03824 2.66418
H 2.53781 2.97666 0.13731
H 4.96820 2.93602 0.02815
H 4.97756 1.11411 0.36671
H -3.31133 -0.44853 0.86660
H -2.40233 -1.91515 0.57779
H -0.35191 1.99879 1.27450
H -1.94560 1.62244 1.88542
H -1.43106 2.38530 -1.06113
H -2.07575 -1.19201 -1.86900
H -3.42665 3.72066 -0.79482
H -3.58771 3.18467 0.97212
H -4.18061 -0.45401 -2.78570
H -4.81843 -0.05469 -1.09251
45
bora-aza-Cope_TS-cis-2-conf15 E=-743.013667088 G=-742.699208 Imag-freq=1
C 1.76398 -0.42478 1.76032
C 1.16615 -0.56201 0.38012
N -0.00696 0.34093 0.21874
C 0.06662 1.59140 0.73213
C 1.08409 1.95054 1.81073
C 1.73502 0.73608 2.41601
C 2.26787 -0.37697 -0.70834
C 0.53885 2.81461 -0.89652
C -0.51845 2.42419 -1.71748
C -0.65164 1.12279 -2.25832
C 3.29803 -1.47445 -0.67170
C 4.61609 -1.29209 -0.53831
B -1.13502 0.01671 -0.75693
C -2.62235 0.58256 -0.32509

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C     -1.12562    -1.47278    -1.42795
C     -1.39345    -2.73316    -0.63271
C     -3.20827     0.09474     0.97047
C     -1.47476    -2.88267     0.69537
C     -4.42452    -0.44267     1.14128
H      2.25475    -1.29905     2.17835
H      0.77643    -1.57472     0.27042
H     -0.89594     2.06145     0.87974
H      0.56862     2.53485     2.58165
H      1.86301     2.61652     1.41705
H      2.19356     0.84467     3.39588
H      2.75831     0.59458    -0.59055
H      1.78440    -0.38934    -1.69130
H      1.52496     2.38664    -1.04912
H      0.53528     3.81624    -0.47298
H     -1.40954     3.05213    -1.69831
H     -1.48938     0.96789    -2.93865
H      0.26137     0.64306    -2.60539
H      2.91354    -2.49023    -0.77837
H      5.30783    -2.12992    -0.53862
H      5.04619    -0.29876    -0.42756
H     -3.32422     0.35533    -1.14024
H     -2.59580     1.68070    -0.26865
H     -0.18128    -1.64957    -1.97065
H     -1.87283    -1.44980    -2.23760
H     -1.50717    -3.63502    -1.24055
H     -2.57996     0.21798     1.85590
H     -1.65326    -3.85836     1.14120
H     -1.38138    -2.04430     1.37945
H     -4.77686    -0.76087     2.11942
H     -5.10264    -0.59415     0.30275
45
bora-aza-Cope_TS-cis-2-conf16 E=-743.017314045 G=-742.701863 Imag-freq=1
C     -1.98345     1.52391     1.44365
C     -1.07564     1.22074     0.27743
N     -0.25183     0.00864     0.52743
C     -0.76929    -1.02639     1.23728
C     -2.05191    -0.86996     2.05057
C     -2.43033     0.57097     2.26183
C     -1.87249     1.27751    -1.06671
C     -1.17447    -2.50039    -0.13090
C      0.06854    -2.53562    -0.76673
C      0.58449    -1.44976    -1.51626
C     -3.10636     0.42504    -1.19320
C     -3.43005    -0.29224    -2.27528
B      1.08274    -0.19840    -0.19054
C      2.23790    -0.88955     0.76464
C      1.66182     1.07827    -1.04467
C      2.24662     2.18908    -0.21947
C      3.52626    -1.24079     0.08029
C      1.88362     3.48097    -0.24427
C      4.74079    -0.74308     0.35611
H     -2.28367     2.56193     1.56675
H     -0.35290     2.03579     0.20598
H     -0.02290    -1.62261     1.74473
H     -1.91084    -1.37715     3.01152
H     -2.89087    -1.38926     1.56893
H     -3.10108     0.80233     3.08586
H     -1.19716     1.08649    -1.90515
H     -2.18099     2.32997    -1.15854
H     -1.99095    -1.96041    -0.59907
H     -1.47133    -3.34824     0.48306
H      0.77723    -3.29482    -0.43421
H      1.51815    -1.63167    -2.04858
H     -0.13102    -0.88750    -2.11394
H     -3.79651     0.44608    -0.35023
H     -4.35899    -0.85357    -2.32627
H     -2.77846    -0.34336    -3.14542
H      1.85623    -1.81134     1.22502
H      2.45209    -0.20243     1.59739
H      0.93198     1.49372    -1.75064
H      2.47246     0.66077    -1.66103
H      3.04385     1.90077     0.46695
H      3.45550    -1.97836    -0.72242
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H      2.35787     4.21836     0.39853
H      1.10185     3.84306    -0.91027
H      5.62297    -1.05113    -0.19949
H      4.89032    -0.00816     1.14539
45
bora-aza-Cope_TS-cis-2-conf17 E=-743.021969328 G=-742.708516 Imag-freq=1
C      2.21894    -0.83235    -1.39383
C      1.27822     0.16717    -0.76360
N      0.14734    -0.51419    -0.08415
C      0.39192    -1.65754     0.60542
C      1.67817    -2.45278     0.38964
C      2.40828    -2.03916    -0.85969
C      2.06439     1.15061     0.15797
C      0.42474    -1.11301     2.58190
C     -0.82772    -0.49625     2.61789
C     -1.12356     0.69891     1.91858
C      3.02914     2.01654    -0.60679
C      4.34207     2.10658    -0.36910
B     -1.20729     0.17062     0.11338
C     -2.50154    -0.84121    -0.01344
C     -1.38210     1.56448    -0.74074
C     -2.68264     2.28498    -0.54001
C     -2.73855    -1.33494    -1.41016
C     -2.83836     3.50118     0.00355
C     -2.69337    -2.61193    -1.82034
H      2.76337    -0.51190    -2.27746
H      0.83246     0.76504    -1.56203
H     -0.47930    -2.28832     0.72013
H      1.41929    -3.51670     0.35157
H      2.35560    -2.34954     1.24732
H      3.10778    -2.74828    -1.29564
H      2.59968     0.58893     0.93061
H      1.33900     1.79898     0.66224
H      1.31808    -0.49862     2.51175
H      0.56101    -2.05597     3.10655
H     -1.66929    -1.10852     2.94328
H     -2.11273     1.12508     2.08449
H     -0.34245     1.45806     1.90601
H      2.59497     2.61965    -1.40615
H      4.97989     2.76742    -0.94957
H      4.82094     1.52459     0.41570
H     -3.38273    -0.27088     0.31669
H     -2.43888    -1.70257     0.66277
H     -1.30488     1.30218    -1.80926
H     -0.56363     2.26624    -0.53599
H     -3.58161     1.75946    -0.86707
H     -2.94470    -0.57069    -2.16267
H     -3.82092     3.95012     0.12434
H     -1.98606     4.08488     0.34766
H     -2.85094    -2.88320    -2.86120
H     -2.49717    -3.42691    -1.12541
45
bora-aza-Cope_TS-cis-2-conf18 E=-743.020638580 G=-742.705944 Imag-freq=1
C      2.41310     0.21399    -1.52985
C      1.46261     0.53795    -0.40137
N      0.24750    -0.31737    -0.46196
C      0.39657    -1.62724    -0.78517
C      1.66479    -2.13797    -1.46612
C      2.51224    -1.02313    -2.01677
C      2.20554     0.48413     0.96926
C      0.29025    -2.65068     0.99670
C     -0.93153    -2.13044     1.42659
C     -1.11767    -0.77238     1.78160
C      3.26914     1.54238     1.09170
C      4.55926     1.31341     1.35889
B     -1.09172     0.13639     0.13276
C     -2.39459    -0.36618    -0.74190
C     -1.18147     1.72123     0.55382
C     -1.37267     2.67483    -0.59350
C     -3.72977    -0.09262    -0.11782
C     -2.41499     3.49842    -0.77703
C     -4.63892    -1.01042     0.24471
H      3.03989     1.02092    -1.89839
H      1.11728     1.56458    -0.53329
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H     -0.50191    -2.08470    -1.17556
H      1.36801    -2.82719    -2.26457
H      2.27117    -2.73867    -0.77575
H      3.21799    -1.26643    -2.80725
H      2.64768    -0.50665     1.11600
H      1.46744     0.63920     1.76414
H      1.21297    -2.25068     1.40743
H      0.34039    -3.69415     0.69414
H     -1.82491    -2.71128     1.19493
H     -2.10196    -0.51258     2.17058
H     -0.30817    -0.29833     2.33496
H      2.93156     2.57202     0.96077
H      5.27270     2.12753     1.45201
H      4.94294     0.30454     1.49626
H     -2.35027    -1.43077    -1.00092
H     -2.33950     0.18818    -1.69362
H     -0.28393     2.01752     1.11627
H     -2.01829     1.84559     1.25360
H     -0.59040     2.68113    -1.35621
H     -3.96822     0.95640     0.06363
H     -2.48360     4.14617    -1.64735
H     -3.23480     3.54882    -0.06239
H     -5.58028    -0.72848     0.70975
H     -4.46908    -2.07465     0.08830
45
bora-aza-Cope_TS-cis-2-conf19 E=-743.011997336 G=-742.696704 Imag-freq=1
C     -1.07204     1.09336     2.08459
C     -0.55955     1.11689     0.66611
N     -0.00955    -0.20320     0.26322
C     -0.56048    -1.34577     0.73828
C     -1.50989    -1.33705     1.93247
C     -1.50586    -0.02446     2.66746
C     -1.61305     1.77360    -0.28553
C     -1.66848    -2.11889    -0.82929
C     -0.65453    -2.12237    -1.78789
C     -0.04633    -0.94380    -2.28491
C     -3.01463     1.22527    -0.27588
C     -3.75797     1.01454    -1.36817
B      1.03790    -0.32453    -0.83791
C      2.17274    -1.48961    -0.61414
C      1.65369     1.07605    -1.44337
C      2.68704     1.78166    -0.61257
C      2.99583    -1.54488     0.65495
C      2.62610     3.04999    -0.17738
C      2.88997    -0.79097     1.75751
H     -1.10130     2.04862     2.60376
H      0.29813     1.79320     0.63728
H      0.12557    -2.18254     0.74543
H     -1.21964    -2.15324     2.60429
H     -2.53774    -1.56870     1.62380
H     -1.89166    -0.01571     3.68417
H     -1.22632     1.79539    -1.30785
H     -1.66203     2.82274     0.04327
H     -2.39434    -1.31275    -0.82231
H     -2.02917    -3.07155    -0.44686
H     -0.11825    -3.06019    -1.93480
H      0.68212    -1.08000    -3.08491
H     -0.69998    -0.08965    -2.45369
H     -3.45418     1.03985     0.70373
H     -4.78279     0.66059    -1.29683
H     -3.36759     1.18682    -2.36930
H      2.88456    -1.41513    -1.45398
H      1.75585    -2.50061    -0.74176
H      0.87410     1.79332    -1.72954
H      2.13924     0.77389    -2.38461
H      3.56176     1.19123    -0.33935
H      3.76393    -2.32366     0.66220
H      3.41705     3.48313     0.42990
H      1.78176     3.69565    -0.41440
H      3.54683    -0.95110     2.60939
H      2.15619     0.00407     1.84643
45
bora-aza-Cope_TS-cis-2-conf1 E=-743.019758614 G=-742.705583 Imag-freq=1
C     -1.74614     0.16809     1.80090
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C     -1.12169     0.45652     0.45665
N      0.04455    -0.43095     0.20818
C     -0.03088    -1.73025     0.58878
C     -1.06520    -2.20003     1.60879
C     -1.72741    -1.05635     2.32849
C     -2.20266     0.40558    -0.66692
C     -0.45684    -2.78069    -1.13916
C      0.61940    -2.31519    -1.89592
C      0.75674    -0.96886    -2.31157
C     -3.24406     1.48244    -0.51769
C     -4.56262     1.27471    -0.43564
B      1.18202    -0.01203    -0.71936
C      2.66948    -0.56060    -0.26716
C      1.17618     1.54810    -1.23415
C      1.56371     2.60003    -0.23247
C      3.12550    -0.16228     1.10869
C      0.83539     3.67221     0.11615
C      4.25782     0.48505     1.42034
H     -2.24605     0.99220     2.30191
H     -0.72125     1.47161     0.47439
H      0.93381    -2.20312     0.71586
H     -0.56205    -2.86318     2.32175
H     -1.83767    -2.81893     1.13418
H     -2.20413    -1.26900     3.28231
H     -2.68554    -0.57696    -0.67835
H     -1.69995     0.53988    -1.63126
H     -1.44145    -2.34605    -1.28455
H     -0.45988    -3.81829    -0.81329
H      1.51475    -2.93731    -1.90810
H      1.61109    -0.74972    -2.95265
H     -0.15098    -0.46588    -2.64104
H     -2.86881     2.50675    -0.49116
H     -5.26294     2.10075    -0.34792
H     -4.98445     0.27191    -0.45655
H      3.40972    -0.22050    -1.00531
H      2.69512    -1.65911    -0.31532
H      0.22198     1.82959    -1.70035
H      1.92121     1.57276    -2.04509
H      2.52967     2.46109     0.25159
H      2.45888    -0.43883     1.92888
H      1.18942     4.38451     0.85733
H     -0.13817     3.87303    -0.32867
H      4.50810     0.73525     2.44832
H      4.96722     0.79356     0.65391
45
bora-aza-Cope_TS-cis-2-conf20 E=-743.017980835 G=-742.703999 Imag-freq=1
C      1.83741     0.19300    -1.83176
C      1.15162     0.57441    -0.54144
N      0.11591    -0.42467    -0.16963
C      0.38362    -1.73953    -0.36103
C      1.48871    -2.19779    -1.30915
C      2.00093    -1.08344    -2.18057
C      2.20641     0.83638     0.57788
C      0.92922    -2.46125     1.50203
C     -0.22899    -2.06926     2.17336
C     -0.58602    -0.71706     2.39443
C      3.06894     2.03567     0.28832
C      4.40460     2.02810     0.22363
B     -1.09822    -0.05403     0.68345
C     -2.47829    -0.85911     0.27892
C     -1.31296     1.54313     0.99022
C     -1.93257     2.38568    -0.09081
C     -2.84337    -0.83274    -1.18020
C     -3.03594     3.13705     0.03473
C     -4.00642    -0.43164    -1.71265
H      2.22854     1.00154    -2.44253
H      0.61910     1.51378    -0.70239
H     -0.50088    -2.36036    -0.41006
H      1.09143    -3.01395    -1.92354
H      2.32994    -2.63586    -0.75658
H      2.52376    -1.35726    -3.09371
H      2.83521    -0.04947     0.71271
H      1.67178     1.00985     1.51858
H      1.82984    -1.86057     1.58864
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H      1.10139    -3.52044     1.32563
H     -1.01815    -2.81642     2.26267
H     -1.48535    -0.55186     2.98827
H      0.22144    -0.03764     2.66398
H      2.53797     2.97689     0.13563
H      4.96840     2.93593     0.02766
H      4.97743     1.11429     0.36767
H     -3.31123    -0.44826     0.86664
H     -2.40230    -1.91503     0.57848
H     -0.35207     1.99927     1.27381
H     -1.94554     1.62269     1.88516
H     -1.43171     2.38533    -1.06155
H     -2.07576    -1.19321    -1.86858
H     -3.42792     3.71975    -0.79518
H     -3.58858     3.18380     0.97181
H     -4.18033    -0.45506    -2.78571
H     -4.81805    -0.05450    -1.09279
45
bora-aza-Cope_TS-cis-2-conf21 E=-743.021969344 G=-742.708511 Imag-freq=1
C      2.21878    -0.83231    -1.39395
C      1.27824     0.16728    -0.76354
N      0.14738    -0.51408    -0.08405
C      0.39207    -1.65734     0.60564
C      1.67847    -2.45237     0.38997
C      2.40825    -2.03903    -0.85967
C      2.06462     1.15051     0.15807
C      0.42468    -1.11260     2.58204
C     -0.82785    -0.49592     2.61792
C     -1.12377     0.69912     1.91846
C      3.02923     2.01657    -0.60673
C      4.34224     2.10641    -0.36941
B     -1.20734     0.17055     0.11335
C     -2.50146    -0.84144    -0.01345
C     -1.38228     1.56436    -0.74082
C     -2.68294     2.28469    -0.54022
C     -2.73840    -1.33527    -1.41015
C     -2.83888     3.50088     0.00328
C     -2.69303    -2.61227    -1.82028
H      2.76295    -0.51200    -2.27779
H      0.83246     0.76529    -1.56185
H     -0.47907    -2.28824     0.72032
H      1.41986    -3.51637     0.35240
H      2.35605    -2.34856     1.24747
H      3.10760    -2.74825    -1.29568
H      2.60008     0.58865     0.93047
H      1.33939     1.79881     0.66267
H      1.31797    -0.49814     2.51193
H      0.56099    -2.05551     3.10679
H     -1.66937    -1.10820     2.94337
H     -2.11298     1.12521     2.08430
H     -0.34272     1.45831     1.90580
H      2.59488     2.61995    -1.40579
H      4.97996     2.76734    -0.94988
H      4.82129     1.52415     0.41509
H     -3.38273    -0.27121     0.31664
H     -2.43870    -1.70277     0.66279
H     -1.30493     1.30204    -1.80933
H     -0.56392     2.26624    -0.53601
H     -3.58180     1.75903    -0.86735
H     -2.94464    -0.57108    -2.16270
H     -3.82152     3.94969     0.12397
H     -1.98669     4.08471     0.34745
H     -2.85055    -2.88361    -2.86113
H     -2.49673    -3.42719    -1.12531
45
bora-aza-Cope_TS-cis-2-conf22 E=-743.012121303 G=-742.698427 Imag-freq=1
C      1.41895    -0.45505    -2.31317
C      1.09538     0.35500    -1.07218
N      0.28538    -0.47274    -0.13761
C      0.67080    -1.75527     0.06427
C      1.68324    -2.42372    -0.85988
C      1.71162    -1.75191    -2.21232
C      2.45098     0.92934    -0.53029
C      1.53156    -1.76349     1.95710
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C      0.40511    -1.28585     2.62520
C     -0.10898     0.02530     2.46129
C      2.37856     2.08366     0.43196
C      2.77609     3.32795     0.14166
B     -0.86124     0.07046     0.71927
C     -2.17921    -0.92102     0.78732
C     -1.21829     1.65854     0.52862
C     -2.07302     2.05017    -0.64481
C     -2.70323    -1.40335    -0.53717
C     -3.22924     2.72685    -0.58489
C     -3.95360    -1.27662    -1.00404
H      1.46436     0.07605    -3.26026
H      0.47326     1.20399    -1.35372
H     -0.13132    -2.41498     0.36565
H      1.42244    -3.48264    -0.94980
H      2.69354    -2.40276    -0.43123
H      1.99491    -2.34617    -3.07707
H      3.01453     1.25726    -1.41103
H      3.02446     0.10519    -0.08980
H      2.34085    -1.08210     1.71081
H      1.83157    -2.79906     2.09940
H     -0.26255    -2.03571     3.05082
H     -0.95944     0.28369     3.09294
H      0.62280     0.82864     2.40836
H      2.00042     1.87997     1.43105
H      2.71816     4.12822     0.87421
H      3.17250     3.58620    -0.83846
H     -2.98302    -0.39881     1.32501
H     -1.95220    -1.81064     1.39376
H     -0.28380     2.23665     0.48174
H     -1.72490     1.99578     1.44382
H     -1.71120     1.76029    -1.63391
H     -1.98213    -1.92198    -1.17292
H     -3.79418     2.97375    -1.48038
H     -3.65273     3.04591     0.36625
H     -4.24045    -1.66516    -1.97825
H     -4.72766    -0.76789    -0.43206
45
bora-aza-Cope_TS-cis-2-conf23 E=-743.020831968 G=-742.705945 Imag-freq=1
C     -2.22485     0.21216     1.57188
C     -1.31669     0.47981     0.39512
N     -0.13631    -0.42378     0.41466
C     -0.31423    -1.71955     0.77686
C     -1.56768    -2.16777     1.52602
C     -2.34620    -1.01006     2.09066
C     -2.12472     0.43191    -0.93819
C     -0.32594    -2.78574    -0.98055
C      0.88932    -2.32036    -1.48642
C      1.10095    -0.97726    -1.88046
C     -3.16051     1.52070    -1.02706
C     -4.46752     1.32828    -1.23484
B      1.18396    -0.02110    -0.24352
C      2.50804    -0.55029     0.58566
C      1.30847     1.54379    -0.71794
C      1.53222     2.53349     0.39012
C      3.83631    -0.29088    -0.06265
C      0.78429     3.61408     0.66163
C      4.83062     0.46462     0.42660
H     -2.80361     1.04911     1.95219
H     -0.91719     1.49018     0.49534
H      0.58500    -2.19871     1.13963
H     -1.26035    -2.85226     2.32450
H     -2.22757    -2.75783     0.87673
H     -3.02195    -1.21031     2.91862
H     -2.60340    -0.54636    -1.05142
H     -1.42025     0.55517    -1.76837
H     -1.25371    -2.36241    -1.35502
H     -0.39687    -3.81993    -0.65150
H      1.77153    -2.93122    -1.29181
H      2.06333    -0.75643    -2.34148
H      0.27572    -0.48608    -2.39339
H     -2.78699     2.54096    -0.92433
H     -5.15964     2.16268    -1.30723
H     -4.88713     0.33009    -1.34222
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H      2.44065    -1.63272     0.76305
H      2.49969    -0.07987     1.58066
H      0.46414     1.87223    -1.33822
H      2.19213     1.57358    -1.37351
H      2.39274     2.33902     1.03169
H      3.99931    -0.77186    -1.02970
H      1.01703     4.27332     1.49412
H     -0.08408     3.87529     0.05878
H      5.76134     0.60429    -0.11750
H      4.74336     0.97043     1.38678
45
bora-aza-Cope_TS-cis-2-conf24 E=-743.017980831 G=-742.704012 Imag-freq=1
C     -1.83721     0.19319     1.83183
C     -1.15162     0.57439     0.54134
N     -0.11586    -0.42467     0.16964
C     -0.38353    -1.73950     0.36123
C     -1.48866    -2.19763     1.30936
C     -2.00068    -1.08321     2.18082
C     -2.20654     0.83600    -0.57794
C     -0.92905    -2.46153    -1.50177
C      0.22913    -2.06956    -2.17314
C      0.58613    -0.71738    -2.39440
C     -3.06901     2.03542    -0.28871
C     -4.40466     2.02787    -0.22371
B      1.09827    -0.05410    -0.68352
C      2.47836    -0.85906    -0.27882
C      1.31284     1.54304    -0.99048
C      1.93209     2.38580     0.09061
C      2.84349    -0.83223     1.18027
C      3.03527     3.13747    -0.03481
C      4.00675    -0.43137     1.71245
H     -2.22818     1.00182     2.44259
H     -0.61920     1.51386     0.70201
H      0.50099    -2.36028     0.41041
H     -1.09153    -3.01390     1.92369
H     -2.33000    -2.63551     0.75679
H     -2.52331    -1.35693     3.09409
H     -2.83540    -0.04987    -0.71240
H     -1.67202     1.00913    -1.51876
H     -1.82972    -1.86094    -1.58845
H     -1.10114    -3.52071    -1.32520
H      1.01834    -2.81670    -2.26231
H      1.48549    -0.55228    -2.98824
H     -0.22128    -0.03795    -2.66407
H     -2.53801     2.97670    -0.13653
H     -4.96842     2.93578    -0.02799
H     -4.97752     1.11400    -0.36724
H      3.31128    -0.44845    -0.86675
H      2.40228    -1.91508    -0.57802
H      0.35192     1.99900    -1.27429
H      1.94557     1.62261    -1.88530
H      1.43111     2.38532     1.06129
H      2.07574    -1.19202     1.86884
H      3.42698     3.72030     0.79514
H      3.58801     3.18435    -0.97182
H      4.18070    -0.45429     2.78552
H      4.81852    -0.05495     1.09234
45
bora-aza-Cope_TS-cis-2-conf25 E=-743.015181637 G=-742.700520 Imag-freq=1
C      2.30568    -0.41893    -1.77449
C      1.57985     0.17919    -0.58440
N      0.25946    -0.48802    -0.42201
C      0.21244    -1.83783    -0.54679
C      1.39304    -2.60949    -1.12878
C      2.23269    -1.72710    -2.02160
C      2.56678     0.12028     0.63482
C     -0.03840    -2.55174     1.37223
C     -1.19451    -1.82555     1.66026
C     -1.21845    -0.41457     1.79413
C      2.29378     1.04598     1.78903
C      3.07937     2.07500     2.12749
B     -1.00587     0.23864     0.04322
C     -2.35525    -0.20605    -0.80262
C     -0.87338     1.86359     0.22391
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C     -0.89901     2.65990    -1.05096
C     -3.63950     0.41919    -0.34626
C      0.02740     3.53858    -1.46381
C     -4.69916    -0.22711     0.16320
H      2.92877     0.24666    -2.36629
H      1.36910     1.22769    -0.79012
H     -0.74332    -2.21827    -0.87942
H      1.00475    -3.47298    -1.67730
H      2.03072    -3.02336    -0.33696
H      2.78009    -2.19008    -2.83851
H      3.55940     0.36080     0.23765
H      2.62210    -0.91665     0.98703
H      0.91957    -2.20182     1.74682
H     -0.11069    -3.62867     1.23843
H     -2.14635    -2.32548     1.47772
H     -2.17475     0.01828     2.08806
H     -0.37906     0.03374     2.32140
H      1.41216     0.84708     2.39351
H      2.84897     2.70954     2.97884
H      3.97857     2.31608     1.56372
H     -2.49671    -1.29313    -0.82294
H     -2.17227     0.09861    -1.84664
H      0.00642     2.14892     0.81286
H     -1.74458     2.16454     0.82619
H     -1.75948     2.49615    -1.70236
H     -3.70550     1.50579    -0.42792
H     -0.06860     4.06421    -2.41053
H      0.91097     3.76084    -0.86784
H     -5.58905     0.30502     0.48972
H     -4.70836    -1.31061     0.27075
45
bora-aza-Cope_TS-cis-2-conf26 E=-743.021709797 G=-742.708055 Imag-freq=1
C      2.25517    -0.63730    -1.55346
C      1.28306     0.23481    -0.79507
N      0.23693    -0.58059    -0.12659
C      0.59542    -1.75678     0.44838
C      1.91636    -2.44029     0.10020
C      2.55243    -1.86885    -1.13816
C      2.04769     1.19042     0.17259
C      0.69955    -1.37740     2.46385
C     -0.58960    -0.86179     2.61133
C     -1.00580     0.36343     2.03562
C      2.90658     2.18792    -0.55732
C      4.22139     2.35303    -0.37744
B     -1.14707    -0.00413     0.19783
C     -2.37714    -1.08489     0.02628
C     -1.45107     1.44276    -0.51786
C     -2.77027     2.06440    -0.16836
C     -2.61489    -1.48914    -1.39984
C     -2.95221     3.22351     0.48191
C     -3.72779    -1.27823    -2.11850
H      2.73089    -0.20409    -2.42865
H      0.75670     0.86440    -1.51619
H     -0.22308    -2.45604     0.55439
H      1.72290    -3.51155    -0.02471
H      2.62985    -2.36985     0.93153
H      3.27482    -2.48607    -1.66672
H      2.66254     0.60574     0.86473
H      1.30737     1.73704     0.76746
H      1.54221    -0.69426     2.40381
H      0.92998    -2.34852     2.89605
H     -1.36740    -1.56100     2.92013
H     -2.01200     0.69826     2.28635
H     -0.28247     1.17788     2.05718
H      2.38803     2.82418    -1.27669
H      4.77921     3.10649    -0.92661
H      4.78173     1.74192     0.32718
H     -3.29838    -0.65745     0.44363
H     -2.18237    -1.99268     0.61474
H     -1.44220     1.26474    -1.60615
H     -0.65871     2.17387    -0.31314
H     -3.65821     1.50897    -0.47339
H     -1.77841    -1.98871    -1.89457
H     -3.94643     3.60068     0.70790
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H     -2.11049     3.83072     0.81134
H     -3.80344    -1.58745    -3.15806
H     -4.59905    -0.78602    -1.68932
45
bora-aza-Cope_TS-cis-2-conf27 E=-743.017002864 G=-742.704178 Imag-freq=1
C      2.62214    -0.62238    -1.40483
C      1.54090     0.20835    -0.75682
N      0.34067    -0.60690    -0.43757
C      0.51903    -1.87738     0.01371
C      1.85060    -2.60805    -0.15924
C      2.76943    -1.91793    -1.12864
C      2.10883     0.98689     0.47004
C      0.22120    -1.79809     2.02836
C     -1.05506    -1.23223     1.99046
C     -1.30909     0.08548     1.53919
C      3.15043     2.00273     0.08478
C      4.39655     2.05262     0.56761
B     -1.06329     0.01614    -0.31432
C     -2.21349    -0.98399    -0.96072
C     -1.15137     1.57521    -0.84276
C     -2.25395     2.43185    -0.28656
C     -3.63471    -0.50838    -0.96702
C     -2.08383     3.56547     0.41004
C     -4.64389    -1.01598    -0.24267
H      3.29970    -0.10731    -2.07988
H      1.21364     0.95181    -1.48718
H     -0.33011    -2.52333    -0.16213
H      1.63631    -3.63003    -0.49175
H      2.36799    -2.71929     0.80246
H      3.56684    -2.50568    -1.57694
H      2.52707     0.28088     1.19504
H      1.27598     1.50649     0.95759
H      1.07699    -1.16575     2.24822
H      0.32633    -2.83268     2.34719
H     -1.89944    -1.92157     2.02155
H     -2.34008     0.42775     1.62612
H     -0.59267     0.84952     1.83979
H      2.83482     2.75622    -0.63907
H      5.09451     2.82588     0.25871
H      4.75786     1.32332     1.28979
H     -2.19602    -1.97357    -0.48913
H     -1.90090    -1.13367    -2.00794
H     -1.27179     1.52475    -1.93927
H     -0.21519     2.11585    -0.66556
H     -3.27582     2.09750    -0.46074
H     -3.86127     0.32676    -1.63152
H     -2.92981     4.13152     0.79189
H     -1.09217     3.96097     0.62455
H     -5.64888    -0.60537    -0.29750
H     -4.49448    -1.85849     0.43070
45
bora-aza-Cope_TS-cis-2-conf28 E=-743.018043865 G=-742.703391 Imag-freq=1
C      1.98265    -1.20697    -1.83750
C      1.02795    -0.13305    -1.37633
N      0.29935    -0.54034    -0.14767
C      0.92485    -1.30069     0.78721
C      2.25076    -1.99581     0.48778
C      2.54265    -2.06742    -0.98705
C      1.73695     1.26103    -1.35107
C      1.31662    -0.04946     2.36366
C      0.02710     0.46031     2.53016
C     -0.61851     1.26486     1.55816
C      3.01710     1.38502    -0.56949
C      3.31954     2.40643     0.23999
B     -1.07083     0.05434     0.20464
C     -2.12384    -1.03333     0.85582
C     -1.74743     0.94978    -0.99608
C     -3.05366     1.60004    -0.64967
C     -2.56685    -2.08483    -0.11977
C     -3.29113     2.91920    -0.59396
C     -3.81841    -2.30685    -0.54868
H      2.21803    -1.22424    -2.89901
H      0.25412    -0.03420    -2.14171
H      0.25179    -1.91606     1.36925
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H      2.21805    -2.99960     0.92553
H      3.08496    -1.48671     0.98822
H      3.24593    -2.82317    -1.32847
H      1.02751     2.02880    -1.03057
H      1.96444     1.47597    -2.40605
H      2.05372     0.54097     1.82913
H      1.71915    -0.71280     3.12649
H     -0.60202    -0.01393     3.28403
H     -1.58624     1.68055     1.83871
H      0.00727     1.98645     1.03393
H      3.75680     0.60048    -0.72604
H      4.28032     2.46501     0.74403
H      2.61807     3.21727     0.42647
H     -3.00248    -0.50280     1.24610
H     -1.67745    -1.53714     1.72461
H     -1.92982     0.25995    -1.83703
H     -1.06562     1.72359    -1.36852
H     -3.87994     0.92624    -0.41912
H     -1.77235    -2.71504    -0.52707
H     -4.26776     3.31191    -0.32232
H     -2.51373     3.64859    -0.81622
H     -4.04345    -3.08178    -1.27729
H     -4.65867    -1.71718    -0.18555
45
bora-aza-Cope_TS-cis-2-conf29 E=-743.020638636 G=-742.705941 Imag-freq=1
C      2.41318     0.21337    -1.52977
C      1.46271     0.53759    -0.40136
N      0.24745    -0.31752    -0.46194
C      0.39630    -1.62746    -0.78501
C      1.66437    -2.13845    -1.46606
C      2.51208    -1.02379    -2.01666
C      2.20575     0.48381     0.96925
C      0.29000    -2.65062     0.99699
C     -0.93170    -2.13020     1.42693
C     -1.11768    -0.77207     1.78174
C      3.26891     1.54251     1.09173
C      4.55920     1.31404     1.35854
B     -1.09170     0.13642     0.13279
C     -2.39464    -0.36603    -0.74184
C     -1.18123     1.72132     0.55368
C     -1.37215     2.67483    -0.59376
C     -3.72978    -0.09226    -0.11777
C     -2.41431     3.49857    -0.77748
C     -4.63913    -1.00991     0.24463
H      3.04016     1.02015    -1.89832
H      1.11754     1.56426    -0.53338
H     -0.50228    -2.08481    -1.17528
H      1.36738    -2.82752    -2.26456
H      2.27062    -2.73936    -0.77576
H      3.21782    -1.26724    -2.80710
H      2.64834    -0.50680     1.11575
H      1.46774     0.63837     1.76430
H      1.21280    -2.25073     1.40765
H      0.33998    -3.69414     0.69453
H     -1.82515    -2.71098     1.19542
H     -2.10192    -0.51211     2.17073
H     -0.30813    -0.29798     2.33499
H      2.93085     2.57203     0.96116
H      5.27229     2.12845     1.45170
H      4.94336     0.30530     1.49554
H     -2.35047    -1.43064    -1.00080
H     -2.33949     0.18826    -1.69361
H     -0.28369     2.01751     1.11619
H     -2.01809     1.84590     1.25337
H     -0.58979     2.68092    -1.35638
H     -3.96801     0.95679     0.06380
H     -2.48272     4.14623    -1.64788
H     -3.23419     3.54918    -0.06294
H     -5.58045    -0.72783     0.70967
H     -4.46950    -2.07416     0.08811
45
bora-aza-Cope_TS-cis-2-conf2 E=-743.020328258 G=-742.705961 Imag-freq=1
C      1.82364    -0.16728    -1.79283
C      1.18527     0.45526    -0.57422
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N      0.02710    -0.34827    -0.10597
C      0.11360    -1.70163    -0.13574
C      1.14873    -2.41195    -1.00502
C      1.81401    -1.48645    -1.98671
C      2.25806     0.71931     0.52745
C      0.55855    -2.25886     1.79520
C     -0.52976    -1.63712     2.40934
C     -0.70082    -0.23295     2.46341
C      3.27380     1.74897     0.11033
C      4.59732     1.55999     0.08122
B     -1.12675     0.26815     0.67745
C     -2.60593    -0.39714     0.36681
C     -1.15762     1.90849     0.76501
C     -1.68559     2.63530    -0.43982
C     -2.95744    -0.48130    -1.08978
C     -2.79745     3.38394    -0.48522
C     -3.23416    -1.60309    -1.77308
H      2.32661     0.50251    -2.48438
H      0.78080     1.42810    -0.86128
H     -0.85045    -2.19236    -0.13685
H      0.64546    -3.23122    -1.53126
H      1.91985    -2.89413    -0.39031
H      2.30225    -1.93361    -2.84926
H      2.76307    -0.21624     0.78847
H      1.74435     1.08102     1.42531
H      1.53420    -1.78259     1.82318
H      0.58366    -3.34524     1.75053
H     -1.41183    -2.25475     2.57993
H     -1.56709     0.12200     3.02225
H      0.19118     0.36170     2.65512
H      2.87293     2.72369    -0.17328
H      5.27772     2.35417    -0.21335
H      5.04325     0.60573     0.35409
H     -3.33736     0.25654     0.86769
H     -2.73331    -1.38951     0.81698
H     -0.15482     2.29634     0.99784
H     -1.78577     2.17331     1.62646
H     -1.11189     2.53069    -1.36370
H     -2.96361     0.46289    -1.63533
H     -3.12403     3.86623    -1.40309
H     -3.41937     3.53234     0.39606
H     -3.45715    -1.58320    -2.83704
H     -3.24978    -2.57825    -1.28817
45
bora-aza-Cope_TS-cis-2-conf30 E=-743.013443909 G=-742.698675 Imag-freq=1
C     -1.83451     1.33327    -1.74879
C     -0.92782     0.19253    -1.35749
N     -0.24670     0.45318    -0.06361
C     -0.88740     1.14211     0.91252
C     -2.16402     1.92830     0.62740
C     -2.40011     2.13271    -0.84434
C     -1.67077    -1.17587    -1.50922
C     -1.42451    -0.25980     2.32477
C     -0.16870    -0.84197     2.50415
C      0.50923    -1.55927     1.48717
C     -2.98988    -1.34274    -0.80434
C     -3.35980    -2.43742    -0.12995
B      1.08966    -0.20763     0.28861
C      2.12814     0.72729     1.13750
C      1.80687    -1.00067    -0.96179
C      3.06191    -1.74779    -0.61559
C      2.72158     1.95202     0.47802
C      4.28885    -1.51338    -1.10358
C      2.36223     2.52723    -0.67815
H     -2.03166     1.45218    -2.81159
H     -0.12203     0.14893    -2.09504
H     -0.21720     1.65398     1.59033
H     -2.09438     2.89210     1.14432
H     -3.04108     1.42955     1.06044
H     -3.06853     2.93704    -1.14218
H     -0.99717    -1.99422    -1.24073
H     -1.85236    -1.27275    -2.59026
H     -2.15019    -0.74961     1.68403
H     -1.84593     0.33343     3.13376
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H      0.42723    -0.48683     3.34525
H      1.43921    -2.04211     1.78714
H     -0.10368    -2.19175     0.84657
H     -3.69841    -0.52102    -0.90399
H     -4.34504    -2.51965     0.32073
H     -2.69105    -3.28674    -0.00434
H      2.97091     0.08836     1.44538
H      1.70929     1.06319     2.09922
H      2.04496    -0.27920    -1.75688
H      1.10583    -1.72477    -1.40089
H      2.95259    -2.56338     0.10236
H      3.53440     2.42785     1.03430
H      5.14789    -2.10315    -0.79352
H      4.47291    -0.71997    -1.82601
H      2.86252     3.42286    -1.03893
H      1.56181     2.13228    -1.29697
45
bora-aza-Cope_TS-cis-2-conf31 E=-743.014725155 G=-742.699955 Imag-freq=1
C      2.39479     0.00108    -1.86001
C      1.60352     0.48451    -0.65975
N      0.43701    -0.41347    -0.43634
C      0.64627    -1.75056    -0.52824
C      1.93238    -2.30267    -1.13555
C      2.56372    -1.30369    -2.07511
C      2.61720     0.65338     0.52787
C      0.59912    -2.44665     1.41690
C     -0.65977    -1.93740     1.73517
C     -0.93741    -0.55111     1.84032
C      2.21176     1.56785     1.65202
C      2.79103     2.74763     1.90380
B     -0.93059     0.06761     0.06900
C     -2.19744    -0.64830    -0.70940
C     -1.10736     1.69396     0.19856
C     -1.36536     2.41493    -1.09567
C     -3.55160    -0.33738    -0.14749
C     -2.45255     3.13859    -1.40117
C     -4.41878    -1.22209     0.36818
H      2.86386     0.75571    -2.48595
H      1.19938     1.47171    -0.87975
H     -0.22939    -2.31674    -0.81237
H      1.69607    -3.23784    -1.65224
H      2.66094    -2.56902    -0.35879
H      3.16610    -1.67769    -2.89883
H      3.53991     1.04869     0.08872
H      2.86464    -0.34102     0.91724
H      1.48825    -1.91556     1.74503
H      0.72289    -3.52155     1.30691
H     -1.51026    -2.60702     1.60251
H     -1.94301    -0.29273     2.17173
H     -0.17237     0.05763     2.31756
H      1.41064     1.23416     2.30709
H      2.47230     3.37099     2.73462
H      3.60309     3.12800     1.28706
H     -2.09847    -1.73829    -0.77690
H     -2.15792    -0.26712    -1.74349
H     -0.21873     2.13054     0.67512
H     -1.94039     1.89889     0.88421
H     -0.59349     2.32570    -1.86389
H     -3.84299     0.71389    -0.15364
H     -2.56535     3.61698    -2.37084
H     -3.26603     3.27365    -0.69023
H     -5.37803    -0.91084     0.77430
H     -4.19495    -2.28733     0.40173
45
bora-aza-Cope_TS-cis-2-conf32 E=-743.007446377 G=-742.693323 Imag-freq=1
C      1.26187    -0.28006    -2.34163
C      1.13692     0.30913    -0.94977
N      0.09584    -0.44077    -0.19109
C      0.11011    -1.79126    -0.27061
C      0.91814    -2.50553    -1.34798
C      1.17820    -1.59791    -2.52663
C      2.58216     0.36013    -0.33855
C      0.91382    -2.42394     1.56127
C     -0.01841    -1.77554     2.36900
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C     -0.12138    -0.36615     2.47382
C      2.81702     1.32702     0.79065
C      3.54161     2.44652     0.67967
B     -0.86311     0.21454     0.80074
C     -2.38728    -0.42102     0.82371
C     -0.78837     1.83921     0.93968
C     -1.25258     2.78160    -0.15026
C     -3.17306    -0.40427    -0.45761
C     -1.57829     2.50102    -1.41847
C     -4.41753     0.06614    -0.62264
H      1.48514     0.40412    -3.15615
H      0.77852     1.33448    -1.02659
H     -0.84448    -2.25726    -0.07040
H      0.36899    -3.40166    -1.65324
H      1.87853    -2.86632    -0.95742
H      1.31317    -2.05063    -3.50549
H      3.24740     0.64060    -1.16284
H      2.87652    -0.65288    -0.04121
H      1.88842    -1.97451     1.39593
H      0.89139    -3.50892     1.49105
H     -0.87415    -2.36648     2.69665
H     -0.84914     0.00875     3.19403
H      0.81454     0.18578     2.50651
H      2.38380     1.08519     1.75822
H      3.69259     3.11164     1.52542
H      4.00749     2.73391    -0.26102
H     -2.96353     0.10113     1.60086
H     -2.34396    -1.46867     1.15609
H      0.23469     2.15623     1.19972
H     -1.36587     2.09762     1.84213
H     -1.29452     3.83242     0.14969
H     -2.67865    -0.84312    -1.32769
H     -1.87626     3.28669    -2.10894
H     -1.57450     1.48725    -1.80745
H     -4.91930     0.02995    -1.58655
H     -4.96964     0.51686     0.20074
45
bora-aza-Cope_TS-cis-2-conf33 E=-743.016325803 G=Imag-freq=1
C     -2.27418     0.24508     1.49709
C     -1.33328     0.49182     0.33938
N     -0.13156    -0.37603     0.44837
C     -0.31675    -1.70685     0.80548
C     -1.62080    -2.13430     1.48686
C     -2.40618    -0.97040     2.03037
C     -2.08792     0.36624    -1.01911
C     -0.17500    -2.77114    -0.87429
C      1.06210    -2.29130    -1.40466
C      1.23261    -1.02355    -1.91183
C     -3.16781     1.40196    -1.18370
C     -4.45669     1.14301    -1.43277
B      1.20178     0.08318    -0.00102
C      2.46170    -0.49929     0.85223
C      1.33663     1.60112    -0.56190
C      1.53091     2.61125     0.53557
C      3.89426    -0.09268     0.57927
C      0.77133     3.66904     0.77328
C      4.49090     0.19434    -0.58608
H     -2.86183     1.08723     1.85192
H     -0.97316     1.51875     0.41447
H      0.55056    -2.12036     1.30663
H     -1.37791    -2.84225     2.28655
H     -2.26087    -2.69175     0.78944
H     -3.10130    -1.15847     2.84537
H     -2.51590    -0.63652    -1.12059
H     -1.35680     0.49707    -1.82559
H     -1.08954    -2.44659    -1.36652
H     -0.20691    -3.80746    -0.54219
H      1.95820    -2.86323    -1.16309
H      2.20788    -0.72057    -2.27758
H      0.39056    -0.48395    -2.33111
H     -2.84552     2.44145    -1.10060
H     -5.18278     1.94171    -1.55712
H     -4.82629     0.12354    -1.52300
H      2.45753    -1.59735     0.88102
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H      2.24551    -0.21360     1.89522
H      0.49599     1.90320    -1.19762
H      2.22830     1.63035    -1.20096
H      2.38305     2.43730     1.19399
H      4.53369    -0.07648     1.46500
H      0.98090     4.34388     1.59869
H     -0.08932     3.90677     0.15121
H      5.55146     0.43071    -0.62231
H      3.96559     0.20679    -1.53576
45
bora-aza-Cope_TS-cis-2-conf34 E=-743.013912214 G=-742.699866 Imag-freq=1
C      1.40877     0.08003    -2.35912
C      0.80012     0.73863    -1.14541
N      0.17534    -0.26190    -0.24016
C      0.74373    -1.48403    -0.09466
C      1.80229    -1.99169    -1.06931
C      1.86708    -1.17149    -2.32925
C      1.80653     1.75144    -0.50534
C      1.67519    -1.45256     1.75055
C      0.57254    -1.04899     2.50402
C     -0.04877     0.21661     2.36264
C      3.18810     1.25992    -0.16648
C      3.84562     1.55359     0.96110
B     -0.96825     0.11201     0.70538
C     -2.11419    -1.06095     0.87888
C     -1.58706     1.62475     0.55227
C     -2.57274     1.87135    -0.55733
C     -2.68843    -1.60510    -0.40069
C     -3.81100     2.36487    -0.41258
C     -3.98423    -1.67301    -0.73714
H      1.48720     0.69110    -3.25512
H     -0.02800     1.35991    -1.49211
H      0.04811    -2.25330     0.21280
H      1.57822    -3.03894    -1.30160
H      2.79623    -2.00421    -0.60322
H      2.32520    -1.62565    -3.20454
H      1.35117     2.22117     0.37088
H      1.91024     2.54723    -1.25826
H      2.41891    -0.71955     1.45678
H      2.04615    -2.46844     1.86967
H     -0.00082    -1.83318     2.99908
H     -0.85133     0.43566     3.06757
H      0.61026     1.06876     2.20146
H      3.69045     0.66626    -0.92951
H      4.86214     1.20916     1.13023
H      3.39077     2.14596     1.75260
H     -2.93020    -0.66737     1.50130
H     -1.70456    -1.91327     1.44076
H     -0.77080     2.35535     0.45243
H     -2.08074     1.87268     1.50217
H     -2.24278     1.63158    -1.57062
H     -1.96388    -1.99604    -1.11864
H     -4.46949     2.51506    -1.26453
H     -4.20920     2.62368     0.56734
H     -4.30530    -2.09183    -1.68785
H     -4.76544    -1.29876    -0.07775
45
bora-aza-Cope_TS-cis-2-conf35 E=-743.012121324 G=-742.698427 Imag-freq=1
C      1.41860    -0.45551    -2.31329
C      1.09528     0.35483    -1.07241
N      0.28540    -0.47269    -0.13754
C      0.67088    -1.75514     0.06459
C      1.68328    -2.42375    -0.85950
C      1.71134    -1.75233    -2.21215
C      2.45098     0.92921    -0.53089
C      1.53178    -1.76283     1.95737
C      0.40525    -1.28528     2.62542
C     -0.10905     0.02578     2.46133
C      2.37878     2.08335     0.43158
C      2.77638     3.32766     0.14147
B     -0.86122     0.07065     0.71926
C     -2.17918    -0.92083     0.78747
C     -1.21827     1.65871     0.52837
C     -2.07314     2.05012    -0.64502
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C     -2.70319    -1.40338    -0.53695
C     -3.22944     2.72665    -0.58507
C     -3.95363    -1.27698    -1.00371
H      1.46377     0.07535    -3.26053
H      0.47315     1.20379    -1.35403
H     -0.13119    -2.41483     0.36618
H      1.42262    -3.48273    -0.94906
H      2.69364    -2.40250    -0.43102
H      1.99447    -2.34682    -3.07679
H      3.01419     1.25733    -1.41178
H      3.02470     0.10504    -0.09075
H      2.34089    -1.08129     1.71090
H      1.83201    -2.79830     2.09984
H     -0.26229    -2.03519     3.05113
H     -0.95958     0.28410     3.09291
H      0.62263     0.82921     2.40839
H      2.00075     1.87949     1.43067
H      2.71863     4.12779     0.87420
H      3.17268     3.58607    -0.83865
H     -2.98299    -0.39854     1.32509
H     -1.95216    -1.81034     1.39406
H     -0.28376     2.23679     0.48129
H     -1.72477     1.99611     1.44358
H     -1.71137     1.76018    -1.63412
H     -1.98201    -1.92188    -1.17271
H     -3.79450     2.97338    -1.48053
H     -3.65288     3.04577     0.36607
H     -4.24047    -1.66566    -1.97788
H     -4.72775    -0.76838    -0.43171
45
bora-aza-Cope_TS-cis-2-conf36 E=-743.020831957 G=-742.705946 Imag-freq=1
C     -2.22469     0.21221     1.57201
C     -1.31669     0.47980     0.39512
N     -0.13630    -0.42381     0.41456
C     -0.31424    -1.71957     0.77679
C     -1.56772    -2.16775     1.52591
C     -2.34605    -1.01001     2.09077
C     -2.12489     0.43181    -0.93808
C     -0.32595    -2.78577    -0.98068
C      0.88938    -2.32046    -1.48640
C      1.10112    -0.97740    -1.88050
C     -3.16061     1.52065    -1.02698
C     -4.46765     1.32829    -1.23460
B      1.18398    -0.02112    -0.24357
C      2.50802    -0.55021     0.58572
C      1.30845     1.54375    -0.71807
C      1.53215     2.53352     0.38993
C      3.83634    -0.29077    -0.06248
C      0.78427     3.61420     0.66123
C      4.83062     0.46469     0.42688
H     -2.80333     1.04920     1.95242
H     -0.91716     1.49017     0.49522
H      0.58498    -2.19875     1.13957
H     -1.26046    -2.85243     2.32425
H     -2.22771    -2.75758     0.87652
H     -3.02168    -1.21026     2.91883
H     -2.60365    -0.54646    -1.05113
H     -1.42048     0.55486    -1.76834
H     -1.25364    -2.36235    -1.35519
H     -0.39699    -3.81996    -0.65165
H      1.77154    -2.93134    -1.29164
H      2.06361    -0.75662    -2.34131
H      0.27605    -0.48619    -2.39364
H     -2.78701     2.54090    -0.92441
H     -5.15972     2.16273    -1.30700
H     -4.88734     0.33012    -1.34181
H      2.44066    -1.63264     0.76317
H      2.49957    -0.07974     1.58070
H      0.46411     1.87211    -1.33837
H      2.19211     1.57354    -1.37364
H      2.39256     2.33904     1.03163
H      3.99941    -0.77169    -1.02955
H      1.01696     4.27351     1.49368
H     -0.08400     3.87543     0.05824
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H      5.76138     0.60438    -0.11714
H      4.74329     0.97046     1.38709
45
bora-aza-Cope_TS-cis-2-conf37 E=-743.013667090 G=-742.699212 Imag-freq=1
C     -1.76392     0.42475     1.76036
C     -1.16617     0.56192     0.38012
N      0.00697    -0.34098     0.21875
C     -0.06660    -1.59144     0.73216
C     -1.08415    -1.95059     1.81068
C     -1.73497    -0.73611     2.41604
C     -2.26793     0.37675    -0.70829
C     -0.53870    -2.81467    -0.89655
C      0.51861    -2.42419    -1.71746
C      0.65176    -1.12278    -2.25829
C     -3.29795     1.47436    -0.67188
C     -4.61602     1.29219    -0.53832
B      1.13505    -0.01671    -0.75690
C      2.62240    -0.58250    -0.32505
C      1.12551     1.47279    -1.42792
C      1.39325     2.73320    -0.63270
C      3.20834    -0.09471     0.97050
C      1.47443     2.88277     0.69538
C      4.42450     0.44295     1.14125
H     -2.25461     1.29906     2.17842
H     -0.77650     1.57464     0.27033
H      0.89597    -2.06146     0.87984
H     -0.56877    -2.53504     2.58155
H     -1.86314    -2.61645     1.41690
H     -2.19345    -0.84470     3.39594
H     -2.75848    -0.59472    -0.59026
H     -1.78447     0.38881    -1.69126
H     -1.52482    -2.38672    -1.04916
H     -0.53511    -3.81630    -0.47302
H      1.40973    -3.05208    -1.69825
H      1.48951    -0.96785    -2.93861
H     -0.26126    -0.64310    -2.60542
H     -2.91335     2.49007    -0.77888
H     -5.30766     2.13011    -0.53881
H     -5.04624     0.29895    -0.42725
H      3.32425    -0.35525    -1.14022
H      2.59585    -1.68064    -0.26862
H      0.18112     1.64948    -1.97056
H      1.87268     1.44986    -2.23761
H      1.50697     3.63504    -1.24057
H      2.58015    -0.21819     1.85598
H      1.65286     3.85848     1.14118
H      1.38104     2.04442     1.37948
H      4.77687     0.76112     2.11937
H      5.10250     0.59467     0.30266
45
bora-aza-Cope_TS-cis-2-conf38 E=-743.017980859 G=-742.704009 Imag-freq=1
C      1.83698     0.19340    -1.83189
C      1.15158     0.57443    -0.54125
N      0.11585    -0.42468    -0.16959
C      0.38360    -1.73949    -0.36124
C      1.48881    -2.19746    -1.30937
C      2.00053    -1.08298    -2.18095
C      2.20666     0.83579     0.57793
C      0.92912    -2.46158     1.50170
C     -0.22914    -2.06975     2.17304
C     -0.58624    -0.71761     2.39438
C      3.06895     2.03539     0.28890
C      4.40459     2.02801     0.22367
B     -1.09831    -0.05417     0.68354
C     -2.47839    -0.85912     0.27876
C     -1.31289     1.54296     0.99058
C     -1.93211     2.38582    -0.09045
C     -2.84342    -0.83239    -1.18036
C     -3.03524     3.13756     0.03503
C     -4.00650    -0.43122    -1.71269
H      2.22772     1.00209    -2.44270
H      0.61915     1.51393    -0.70168
H     -0.50088    -2.36034    -0.41050
H      1.09187    -3.01389    -1.92361
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H      2.33028    -2.63506    -0.75678
H      2.52301    -1.35663    -3.09432
H      2.83565    -0.05006     0.71198
H      1.67231     1.00853     1.51892
H      1.82971    -1.86089     1.58848
H      1.10133    -3.52073     1.32510
H     -1.01829    -2.81695     2.26213
H     -1.48563    -0.55261     2.98818
H      0.22112    -0.03815     2.66413
H      2.53781     2.97665     0.13708
H      4.96821     2.93604     0.02811
H      4.97757     1.11416     0.36683
H     -3.31134    -0.44847     0.86661
H     -2.40234    -1.91512     0.57800
H     -0.35197     1.99888     1.27445
H     -1.94563     1.62248     1.88540
H     -1.43112     2.38540    -1.06113
H     -2.07574    -1.19253    -1.86882
H     -3.42691     3.72047    -0.79487
H     -3.58798     3.18440     0.97205
H     -4.18037    -0.45422    -2.78576
H     -4.81820    -0.05444    -1.09269
45
bora-aza-Cope_TS-cis-2-conf3 E=-743.021709795 G=-742.708055 Imag-freq=1
C      2.25505    -0.63730    -1.55360
C      1.28300     0.23481    -0.79514
N      0.23693    -0.58060    -0.12658
C      0.59551    -1.75675     0.44842
C      1.91653    -2.44014     0.10028
C      2.55240    -1.86881    -1.13825
C      2.04766     1.19041     0.17252
C      0.69963    -1.37732     2.46389
C     -0.58957    -0.86183     2.61134
C     -1.00588     0.36334     2.03562
C      2.90662     2.18785    -0.55739
C      4.22140     2.35299    -0.37734
B     -1.14709    -0.00417     0.19784
C     -2.37712    -1.08495     0.02627
C     -1.45108     1.44273    -0.51783
C     -2.77027     2.06438    -0.16829
C     -2.61492    -1.48911    -1.39987
C     -2.95219     3.22353     0.48191
C     -3.72787    -1.27822    -2.11845
H      2.73061    -0.20415    -2.42891
H      0.75659     0.86441    -1.51621
H     -0.22292    -2.45608     0.55446
H      1.72323    -3.51145    -0.02441
H      2.63008    -2.36940     0.93153
H      3.27473    -2.48606    -1.66686
H      2.66244     0.60572     0.86470
H      1.30732     1.73708     0.76733
H      1.54222    -0.69409     2.40383
H      0.93015    -2.34841     2.89610
H     -1.36732    -1.56111     2.92013
H     -2.01211     0.69809     2.28635
H     -0.28263     1.17786     2.05717
H      2.38816     2.82402    -1.27690
H      4.77928     3.10641    -0.92651
H      4.78166     1.74198     0.32742
H     -3.29837    -0.65758     0.44370
H     -2.18229    -1.99278     0.61466
H     -1.44225     1.26473    -1.60611
H     -0.65871     2.17383    -0.31311
H     -3.65823     1.50891    -0.47322
H     -1.77843    -1.98859    -1.89468
H     -3.94639     3.60071     0.70793
H     -2.11045     3.83078     0.81125
H     -3.80355    -1.58737    -3.15803
H     -4.59915    -0.78610    -1.68919
45
bora-aza-Cope_TS-cis-2-conf4 E=-743.020714614 G=-742.706986 Imag-freq=1
C      2.18472    -0.33185    -1.68630
C      1.26989     0.40812    -0.73996
N      0.25437    -0.50063    -0.14997
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C      0.62643    -1.75853     0.19894
C      1.90661    -2.38897    -0.34632
C      2.48300    -1.61823    -1.50272
C      2.10257     1.19186     0.32187
C      0.87540    -1.71269     2.23342
C     -0.39814    -1.23708     2.55072
C     -0.85254     0.06178     2.21516
C      2.92174     2.29865    -0.28591
C      4.24733     2.43146    -0.16974
B     -1.10309     0.01381     0.34112
C     -2.34895    -1.02405     0.06186
C     -1.43561     1.55923    -0.10526
C     -2.64869     2.17552     0.52939
C     -2.55677    -1.32896    -1.39390
C     -3.75625     2.59217    -0.10104
C     -3.64861    -1.05832    -2.12476
H      2.62016     0.23939    -2.50112
H      0.70999     1.14735    -1.31773
H     -0.19857    -2.45705     0.24441
H      1.67813    -3.41827    -0.64517
H      2.66965    -2.47798     0.43780
H      3.16535    -2.14134    -2.16828
H      2.75523     0.50149     0.86618
H      1.40666     1.62989     1.04636
H      1.71615    -1.02480     2.22770
H      1.12912    -2.73985     2.48529
H     -1.15429    -1.98424     2.79365
H     -1.84124     0.32591     2.58990
H     -0.13336     0.87213     2.33078
H      2.36359     3.04674    -0.85162
H      4.77581     3.26669    -0.62092
H      4.84638     1.71070     0.38304
H     -3.26861    -0.59384     0.47943
H     -2.19377    -1.97406     0.59343
H     -1.55679     1.59372    -1.19858
H     -0.58122     2.20936     0.13328
H     -2.60975     2.30003     1.61337
H     -1.71662    -1.80981    -1.90070
H     -4.59063     3.02864     0.44227
H     -3.86508     2.50507    -1.18059
H     -3.70156    -1.30266    -3.18294
H     -4.52263    -0.57872    -1.68777
45
bora-aza-Cope_TS-cis-2-conf5 E=-743.020638570 G=-742.705943 Imag-freq=1
C     -2.41284     0.21408     1.52999
C     -1.46264     0.53784     0.40120
N     -0.24745    -0.31738     0.46182
C     -0.39648    -1.62724     0.78511
C     -1.66484    -2.13794     1.46584
C     -2.51195    -1.02304     2.01694
C     -2.20591     0.48357    -0.96925
C     -0.28986    -2.65080    -0.99668
C      0.93194    -2.13048    -1.42647
C      1.11799    -0.77245    -1.78158
C     -3.26928     1.54204    -1.09185
C     -4.55956     1.31327    -1.35846
B      1.09177     0.13643    -0.13282
C      2.39458    -0.36587     0.74208
C      1.18137     1.72122    -0.55408
C      1.37227     2.67503     0.59312
C      3.72981    -0.09239     0.11807
C      2.41455     3.49863     0.77678
C      4.63898    -1.01022    -0.24433
H     -3.03934     1.02111     1.89879
H     -1.11736     1.56452     0.53274
H      0.50195    -2.08463     1.17569
H     -1.36830    -2.82764     2.26395
H     -2.27141    -2.73807     0.77515
H     -3.21740    -1.26628     2.80770
H     -2.64834    -0.50715    -1.11544
H     -1.46801     0.63808    -1.76442
H     -1.21255    -2.25093    -1.40758
H     -0.33995    -3.69425    -0.69403
H      1.82534    -2.71121    -1.19465
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H      2.10230    -0.51258    -2.17046
H      0.30853    -0.29848    -2.33506
H     -2.93140     2.57166    -0.96155
H     -5.27282     2.12752    -1.45172
H     -4.94354     0.30442    -1.49518
H      2.35028    -1.43041     1.00134
H      2.33937     0.18871     1.69367
H      0.28385     2.01728    -1.11670
H      2.01826     1.84560    -1.25377
H      0.58980     2.68146     1.35562
H      3.96828     0.95662    -0.06345
H      2.48294     4.14652     1.64701
H      3.23454     3.54891     0.06234
H      5.58037    -0.72833    -0.70934
H      4.46912    -2.07444    -0.08784
45
bora-aza-Cope_TS-cis-2-conf6 E=-743.013667123 G=-742.699217 Imag-freq=1
C     -1.76379     0.42513     1.76028
C     -1.16615     0.56203     0.37996
N      0.00696    -0.34093     0.21872
C     -0.06668    -1.59132     0.73227
C     -1.08434    -1.95029     1.81075
C     -1.73493    -0.73566     2.41609
C     -2.26799     0.37664    -0.70832
C     -0.53873    -2.81473    -0.89632
C      0.51859    -2.42434    -1.71727
C      0.65176    -1.12298    -2.25823
C     -3.29803     1.47424    -0.67200
C     -4.61608     1.29208    -0.53823
B      1.13509    -0.01682    -0.75691
C      2.62239    -0.58262    -0.32493
C      1.12564     1.47259    -1.42811
C      1.39350     2.73306    -0.63302
C      3.20824    -0.09471     0.97061
C      1.47458     2.88277     0.69505
C      4.42441     0.44291     1.14142
H     -2.25431     1.29956     2.17829
H     -0.77647     1.57472     0.26994
H      0.89586    -2.06136     0.88007
H     -0.56912    -2.53487     2.58163
H     -1.86346    -2.61596     1.41692
H     -2.19331    -0.84409     3.39605
H     -2.75852    -0.59481    -0.59007
H     -1.78464     0.38854    -1.69135
H     -1.52484    -2.38680    -1.04899
H     -0.53514    -3.81632    -0.47268
H      1.40970    -3.05225    -1.69803
H      1.48949    -0.96813    -2.93859
H     -0.26126    -0.64329    -2.60534
H     -2.91346     2.48993    -0.77925
H     -5.30773     2.12999    -0.53879
H     -5.04626     0.29885    -0.42690
H      3.32431    -0.35546    -1.14007
H      2.59583    -1.68076    -0.26841
H      0.18125     1.64930    -1.97074
H      1.87279     1.44954    -2.23782
H      1.50742     3.63482    -1.24098
H      2.57996    -0.21807     1.85605
H      1.65311     3.85850     1.14077
H      1.38101     2.04451     1.37924
H      4.77669     0.76117     2.11955
H      5.10249     0.59451     0.30289
45
bora-aza-Cope_TS-cis-2-conf7 E=-743.014749708 G=-742.700533 Imag-freq=1
C      1.83727     0.15031    -1.75368
C      1.10486     0.56962    -0.50179
N      0.04803    -0.41135    -0.14218
C      0.29746    -1.73180    -0.30540
C      1.41314    -2.22746    -1.22036
C      1.98887    -1.13414    -2.07758
C      2.11923     0.85760     0.64805
C      0.80327    -2.42200     1.59075
C     -0.36044    -1.99897     2.23188
C     -0.70748    -0.63837     2.41239
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C      3.00238     2.04120     0.35623
C      4.33947     2.02240     0.34558
B     -1.18660    -0.01434     0.66336
C     -2.56555    -0.81817     0.29323
C     -1.40462     1.59249     0.93258
C     -2.02740     2.39636    -0.17355
C     -3.05985    -0.90865    -1.13412
C     -3.19686     3.04994    -0.10949
C     -2.46187    -0.49805    -2.26063
H      2.27361     0.94067    -2.35767
H      0.58526     1.50800    -0.70874
H     -0.59939    -2.33447    -0.35947
H      1.00525    -3.02932    -1.84712
H      2.22182    -2.69548    -0.64431
H      2.54604    -1.42985    -2.96326
H      2.73436    -0.02890     0.83244
H      1.55178     1.06383     1.56229
H      1.71036    -1.83079     1.67437
H      0.96411    -3.48717     1.44177
H     -1.15922    -2.73507     2.32681
H     -1.61635    -0.44842     2.98371
H      0.10039     0.04222     2.67627
H      2.48571     2.98114     0.15429
H      4.91804     2.91996     0.14541
H      4.89859     1.10940     0.53987
H     -3.37448    -0.35094     0.88014
H     -2.55523    -1.85187     0.67329
H     -0.45001     2.06347     1.21091
H     -2.04641     1.68369     1.81970
H     -1.47463     2.44510    -1.11411
H     -4.03375    -1.39482    -1.24366
H     -3.58961     3.60322    -0.95889
H     -3.80202     3.04469     0.79574
H     -2.93659    -0.64049    -3.22869
H     -1.49211    -0.01053    -2.25713
45
bora-aza-Cope_TS-cis-2-conf8 E=-743.020714606 G=-742.706985 Imag-freq=1
C      2.18465    -0.33234    -1.68635
C      1.26996     0.40789    -0.74007
N      0.25435    -0.50066    -0.14993
C      0.62636    -1.75846     0.19933
C      1.90658    -2.38903    -0.34570
C      2.48289    -1.61869    -1.50242
C      2.10273     1.19163     0.32167
C      0.87523    -1.71217     2.23374
C     -0.39831    -1.23641     2.55094
C     -0.85267     0.06235     2.21506
C      2.92165     2.29858    -0.28613
C      4.24725     2.43154    -0.17021
B     -1.10309     0.01394     0.34103
C     -2.34900    -1.02392     0.06195
C     -1.43546     1.55936    -0.10549
C     -2.64850     2.17579     0.52908
C     -2.55667    -1.32935    -1.39373
C     -3.75618     2.59211    -0.10136
C     -3.64839    -1.05884    -2.12482
H      2.62000     0.23864    -2.50139
H      0.71015     1.14714    -1.31791
H     -0.19864    -2.45698     0.24488
H      1.67818    -3.41848    -0.64412
H      2.66964    -2.47764     0.43843
H      3.16511    -2.14205    -2.16792
H      2.75559     0.50128     0.86578
H      1.40688     1.62944     1.04634
H      1.71602    -1.02435     2.22794
H      1.12885    -2.73930     2.48584
H     -1.15449    -1.98348     2.79405
H     -1.84135     0.32662     2.58975
H     -0.13346     0.87270     2.33047
H      2.36331     3.04666    -0.85166
H      4.77554     3.26687    -0.62140
H      4.84649     1.71079     0.38238
H     -3.26867    -0.59348     0.47924
H     -2.19396    -1.97375     0.59388
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H     -1.55659     1.59381    -1.19882
H     -0.58100     2.20939     0.13306
H     -2.60943     2.30070     1.61301
H     -1.71654    -1.81053    -1.90023
H     -4.59054     3.02868     0.44189
H     -3.86512     2.50461    -1.18087
H     -3.70124    -1.30359    -3.18291
H     -4.52240    -0.57896    -1.68813
45
bora-aza-Cope_TS-cis-2-conf9 E=-743.016404409 G=-742.700986 Imag-freq=1
C     -1.38200     0.17730    -2.33323
C     -0.78181    -0.64626    -1.22068
N     -0.10262     0.20981    -0.21434
C     -0.60392     1.43477     0.08414
C     -1.63965     2.10979    -0.81112
C     -1.77380     1.43845    -2.15063
C     -1.81847    -1.69066    -0.68869
C     -1.52298     1.23013     1.90940
C     -0.44243     0.68524     2.60509
C      0.11535    -0.58330     2.30999
C     -3.16970    -1.18974    -0.25471
C     -3.81861    -1.60070     0.84074
B      1.02449    -0.31905     0.66753
C      2.23108     0.76782     0.97570
C      1.59548    -1.82121     0.31830
C      2.56753    -1.92895    -0.82310
C      2.81181     1.41665    -0.24667
C      3.84971    -2.31243    -0.73435
C      2.82946     2.73258    -0.51163
H     -1.51154    -0.32254    -3.29027
H      0.01432    -1.25257    -1.65792
H      0.14184     2.12165     0.46108
H     -1.35112     3.15986    -0.93484
H     -2.62496     2.13530    -0.32754
H     -2.22591     2.00990    -2.95782
H     -1.36625    -2.28734     0.10844
H     -1.97250    -2.37859    -1.53363
H     -2.30506     0.57423     1.54199
H     -1.84310     2.24105     2.15341
H      0.17102     1.37628     3.18354
H      0.91056    -0.92197     2.97483
H     -0.58440    -1.37823     2.05557
H     -3.65864    -0.47993    -0.92119
H     -4.81499    -1.23838     1.07847
H     -3.37638    -2.31086     1.53675
H      3.02523     0.19471     1.47989
H      1.93444     1.55314     1.68177
H      0.76271    -2.51420     0.13200
H      2.09297    -2.19302     1.22451
H      2.19114    -1.66125    -1.81326
H      3.23715     0.74186    -0.98998
H      4.49590    -2.35158    -1.60767
H      4.29429    -2.59370     0.21893
H      3.24972     3.12328    -1.43517
H      2.42709     3.46247     0.18961
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TS_cis-6:

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45
bora-aza-Cope_TS-cis-6-conf10 E=-743.025466953 G=-742.710768 Imag-freq=1
C     1.51293    -2.06270     1.33963
C     0.39604    -1.70954     0.44405
N     0.09046    -0.40710     0.20142
C     1.14423     0.60129     0.51528
C     1.74234     0.32493     1.90535
C     2.13612    -1.11789     2.05850
C     0.96050    -2.51020    -1.40265
C     2.24776     0.71179    -0.57274
C     3.08439     1.95403    -0.41874
C     4.41478     1.97850    -0.28293
C    -0.21252    -2.16467    -2.07910
C    -0.59173    -0.83719    -2.37076
B    -1.12301    -0.09137    -0.65739
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C     -1.34716     1.48169    -1.05331
C     -2.48897    -0.90721    -0.23694
C     -2.87546    -0.81342     1.21395
C     -1.94586     2.38277    -0.00789
C     -4.05329    -0.40679     1.70827
C     -3.05062     3.12853    -0.15314
H      1.75209    -3.11662     1.44176
H     -0.45685    -2.37351     0.51850
H      0.63576     1.56461     0.55714
H      1.01603     0.58956     2.68805
H      2.60550     0.98098     2.05699
H      2.90322    -1.38578     2.78067
H      1.14799    -3.55765    -1.17987
H      1.85086    -1.90189    -1.52265
H      1.75960     0.74334    -1.55301
H      2.89292    -0.17264    -0.55764
H      2.53853     2.89917    -0.43289
H      4.95948     2.91430    -0.19290
H      5.00258     1.06300    -0.26138
H     -0.98961    -2.92820    -2.12714
H     -1.49985    -0.71035    -2.95947
H      0.19912    -0.14549    -2.65516
H     -1.99481     1.51274    -1.94023
H     -0.38893     1.91724    -1.37708
H     -2.38090    -1.97502    -0.47789
H     -3.32248    -0.54974    -0.85765
H     -2.11131    -1.12500     1.92948
H     -1.42631     2.43335     0.95162
H     -4.24341    -0.37866     2.77844
H     -4.86168    -0.07687     1.05795
H     -3.42615     3.75592     0.65139
H     -3.62063     3.12612    -1.08089
45
bora-aza-Cope_TS-cis-6-conf11 E=-743.025466951 G=-742.710768 Imag-freq=1
C     -1.51295     2.06268     1.33960
C     -0.39604     1.70952     0.44404
N     -0.09046     0.40707     0.20140
C     -1.14421    -0.60133     0.51528
C     -1.74234    -0.32495     1.90534
C     -2.13611     1.11787     2.05849
C     -0.96042     2.51019    -1.40264
C     -2.24774    -0.71187    -0.57275
C     -3.08453    -1.95398    -0.41856
C     -4.41495    -1.97827    -0.28305
C      0.21258     2.16462    -2.07912
C      0.59179     0.83715    -2.37078
B      1.12300     0.09138    -0.65739
C      1.34718    -1.48168    -1.05331
C      2.48894     0.90722    -0.23689
C      2.87542     0.81334     1.21399
C      1.94592    -2.38273    -0.00790
C      4.05332     0.40686     1.70830
C      3.05063    -3.12856    -0.15320
H     -1.75211     3.11660     1.44173
H      0.45686     2.37347     0.51852
H     -0.63572    -1.56464     0.55715
H     -1.01605    -0.58959     2.68806
H     -2.60551    -0.98099     2.05697
H     -2.90320     1.38576     2.78067
H     -1.14786     3.55765    -1.17986
H     -1.85082     1.90194    -1.52266
H     -1.75956    -0.74365    -1.55300
H     -2.89278     0.17264    -0.55782
H     -2.53877    -2.89918    -0.43233
H     -4.95977    -2.91399    -0.19288
H     -5.00266    -1.06270    -0.26187
H      0.98968     2.92815    -2.12722
H      1.49989     0.71032    -2.95953
H     -0.19905     0.14543    -2.65516
H      1.99482    -1.51272    -1.94024
H      0.38897    -1.91725    -1.37707
H      2.38085     1.97505    -0.47776
H      3.32247     0.54983    -0.85763
H      2.11122     1.12472     1.92955
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H      1.42644    -2.43324     0.95166
H      4.24343     0.37865     2.77846
H      4.86178     0.07714     1.05795
H      3.42619    -3.75594     0.65133
H      3.62057    -3.12622    -1.08099
45
bora-aza-Cope_TS-cis-6-conf12 E=-743.027182857 G=-742.712433 Imag-freq=1
C      1.13943    -2.06189     1.61825
C      0.07735    -1.69761     0.66204
N     -0.05776    -0.41164     0.24008
C      1.11502     0.49020     0.43374
C      1.66894     0.33290     1.86015
C      1.87590    -1.11335     2.21478
C      0.53419    -2.80484    -1.04526
C      2.22698     0.30931    -0.63608
C      3.22155     1.43965    -0.62853
C      4.54341     1.30619    -0.47348
C     -0.57156    -2.39914    -1.79865
C     -0.75962    -1.08397    -2.27373
B     -1.20802    -0.06003    -0.68426
C     -1.23950     1.47019    -1.27276
C     -2.67441    -0.64540    -0.21949
C     -3.16102    -0.18418     1.12601
C     -1.63240     2.55670    -0.31034
C     -4.31687     0.44414     1.38562
C     -0.91650     3.65251    -0.01360
H      1.24313    -3.11361     1.86650
H     -0.85367    -2.23046     0.81414
H      0.72712     1.50364     0.33543
H      0.97918     0.79115     2.58463
H      2.60800     0.88992     1.94057
H      2.60164    -1.37485     2.98084
H      0.57285    -3.82901    -0.68241
H      1.50165    -2.34588    -1.22032
H      1.75067     0.27696    -1.62199
H      2.74938    -0.64248    -0.49437
H      2.80679     2.43859    -0.77419
H      5.20766     2.16577    -0.49550
H      5.00446     0.33198    -0.32336
H     -1.44588    -3.05017    -1.77100
H     -1.63312    -0.91366    -2.90258
H      0.12290    -0.54926    -2.61912
H     -1.99326     1.44818    -2.07550
H     -0.29351     1.74415    -1.76009
H     -2.65144    -1.74467    -0.20062
H     -3.41967    -0.38205    -0.98330
H     -2.49690    -0.39260     1.96799
H     -2.59091     2.42289     0.18980
H     -4.58922     0.74497     2.39423
H     -5.02454     0.68535     0.59389
H     -1.27338     4.38899     0.70213
H      0.04916     3.84926    -0.47704
45
bora-aza-Cope_TS-cis-6-conf13 E=-743.028080879 G=-742.713110 Imag-freq=1
C      1.65537    -2.02108     1.48647
C      0.39901    -1.58319     0.84784
N      0.22225    -0.28018     0.49335
C      1.45311     0.55722     0.38899
C      2.34744     0.33844     1.62138
C      2.56812    -1.12455     1.88644
C      0.32198    -2.66998    -0.91390
C      2.24037     0.35393    -0.93492
C      3.27005     1.42827    -1.16398
C      4.57401     1.21810    -1.37500
C     -0.91278    -2.17925    -1.35033
C     -1.12637    -0.84506    -1.75790
B     -1.11179     0.13823    -0.11534
C     -1.21089     1.69694    -0.61497
C     -2.41533    -0.35058     0.76123
C     -3.74902    -0.13690     0.11127
C     -1.39051     2.70238     0.48869
C     -4.63667    -1.09005    -0.21052
C     -2.44128     3.51861     0.65653
H      1.76679    -3.08329     1.68134
```

H -0.48209 -2.07376 1.24279
H 1.11631 1.59367 0.40473
H 1.88932 0.80490 2.50620
H 3.30085 0.85309 1.46467
H 3.45395 -1.43932 2.43240
H 0.38590 -3.70241 -0.57895
H 1.23683 -2.27180 -1.34112
H 1.52549 0.38023 -1.76445
H 2.72165 -0.62933 -0.95033
H 2.89493 2.45341 -1.16595
H 5.26053 2.04130 -1.55266
H 4.99639 0.21525 -1.38100
H -1.79460 -2.76714 -1.09308
H -2.11792 -0.61095 -2.14303
H -0.32542 -0.36315 -2.31571
H -2.05476 1.78682 -1.31131
H -0.31739 1.96264 -1.19909
H -2.38294 0.25147 1.68472
H -2.34899 -1.39942 1.07439
H -4.00555 0.89636 -0.12756
H -0.59139 2.75532 1.23176
H -5.57858 -0.85148 -0.69813
H -4.44788 -2.14101 0.00325
H -2.50092 4.20579 1.49673
H -3.27697 3.52332 -0.04124
45
bora-aza-Cope_TS-cis-6-conf14 E=-743.028158851 G=-742.713091 Imag-freq=1
C 1.57051 -2.05224 1.53964
C 0.32618 -1.67884 0.83938
N 0.11531 -0.39170 0.44936
C 1.31103 0.49822 0.38355
C 2.15894 0.33673 1.65688
C 2.42758 -1.11088 1.95961
C 0.37001 -2.80055 -0.90078
C 2.16345 0.30829 -0.90123
C 3.15633 1.42183 -1.10378
C 4.47660 1.26513 -1.25043
C -0.85974 -2.36946 -1.40934
C -1.10343 -1.05167 -1.85104
B -1.20230 -0.02809 -0.21652
C -1.34092 1.51055 -0.75869
C -2.52269 -0.55566 0.61459
C -3.85054 -0.35269 -0.05439
C -1.57132 2.53961 0.31164
C -4.86022 0.40947 0.39095
C -0.82675 3.63088 0.54709
H 1.71716 -3.10513 1.76009
H -0.55146 -2.19615 1.20781
H 0.92138 1.51562 0.37100
H 1.64405 0.79930 2.51222
H 3.09681 0.88752 1.53226
H 3.30148 -1.37901 2.54817
H 0.45822 -3.82359 -0.54332
H 1.28823 -2.37317 -1.29089
H 1.48537 0.29310 -1.76138
H 2.68567 -0.65396 -0.88057
H 2.73824 2.42933 -1.14275
H 5.13495 2.11427 -1.41206
H 4.94135 0.28171 -1.21754
H -1.72772 -2.99242 -1.19001
H -2.07458 -0.86075 -2.30548
H -0.29104 -0.54550 -2.36855
H -2.22333 1.50930 -1.41636
H -0.49548 1.81699 -1.38890
H -2.53394 -0.04342 1.58879
H -2.43048 -1.62746 0.83908
H -3.99905 -0.88407 -0.99698
H -2.43356 2.36579 0.95698
H -5.78951 0.50639 -0.16473
H -4.78742 0.96374 1.32523
H -1.06433 4.31884 1.35460
H 0.04324 3.87268 -0.06145
45
bora-aza-Cope_TS-cis-6-conf15 E=-743.027982518 G=-742.713670 Imag-freq=1

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C     -1.89901    -2.30109    -0.37151
C     -0.63303    -1.75546     0.15574
N     -0.22953    -0.49968    -0.18194
C     -1.26491     0.41563    -0.74085
C     -2.09883    -0.31136    -1.81014
C     -2.58435    -1.64627    -1.31926
C     -0.91542    -1.73085     2.20160
C     -2.16516     1.07153     0.34275
C     -2.94779     2.24248    -0.18882
C     -4.27902     2.36611    -0.14874
C      0.36758    -1.28110     2.52999
C      0.84569     0.01315     2.23180
B      1.11856    -0.00397     0.32547
C      1.45245     1.55252    -0.06685
C      2.36190    -1.04478     0.06101
C      2.60819    -1.31208    -1.39652
C      2.67399     2.14624     0.57337
C      3.72339    -1.03351    -2.08792
C      3.76330     2.60656    -0.05837
H     -2.20420    -3.27853    -0.01096
H      0.16299    -2.48799     0.22078
H     -0.71797     1.21759    -1.23827
H     -1.49981    -0.45413    -2.72179
H     -2.94108     0.32656    -2.09705
H     -3.47284    -2.08615    -1.76537
H     -1.18531    -2.75749     2.43687
H     -1.74439    -1.03031     2.20165
H     -1.51932     1.42662     1.15358
H     -2.84956     0.33210     0.77167
H     -2.35698     3.04792    -0.62910
H     -4.77963     3.24852    -0.53769
H     -4.91101     1.58996     0.27825
H      1.10888    -2.04594     2.76390
H      1.83790     0.25511     2.61045
H      0.13967     0.83586     2.33485
H      0.59923     2.19107     0.20681
H      1.55802     1.62761    -1.15998
H      2.17796    -2.00709     0.56013
H      3.27388    -0.63879     0.51765
H      1.77771    -1.76977    -1.93919
H      2.65752     2.21480     1.66285
H      3.80466    -1.25001    -3.15034
H      4.58909    -0.57551    -1.61291
H      4.60529     3.02321     0.48871
H      3.84935     2.57593    -1.14308
45
bora-aza-Cope_TS-cis-6-conf16 E=-743.029015824 G=-742.714603 Imag-freq=1
C     -1.89983    -2.36430     0.11755
C     -0.59966    -1.74933     0.44869
N     -0.21454    -0.58747    -0.14823
C     -1.28166     0.21959    -0.80606
C     -2.18245    -0.68632    -1.66329
C     -2.64196    -1.89319    -0.89444
C     -0.73795    -1.33633     2.46897
C     -2.11090     1.08220     0.18543
C     -2.93218     2.13406    -0.51125
C     -4.25711     2.28062    -0.40081
C      0.56042    -0.83684     2.61747
C      1.00040     0.37634     2.04544
B      1.15949    -0.01371     0.18100
C      1.46566     1.43560    -0.52226
C      2.39153    -1.09414     0.04862
C      2.66860    -1.49625    -1.37140
C      2.78704     2.05335    -0.17441
C      3.80244    -1.28721    -2.05701
C      2.97302     3.20916     0.48042
H     -2.18535    -3.24892     0.67839
H      0.19496    -2.47022     0.60027
H     -0.76591     0.90561    -1.47937
H     -1.64062    -1.01204    -2.56367
H     -3.03815    -0.10279    -2.01800
H     -3.55939    -2.39572    -1.19062
H     -0.98184    -2.29905     2.91160
H     -1.57117    -0.64460     2.39499
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H     -1.41400     1.58338     0.86605
H     -2.76225     0.44747     0.79532
H     -2.37656     2.82872    -1.14393
H     -4.78602     3.07512    -0.92003
H     -4.85516     1.61271     0.21595
H      1.32469    -1.54525     2.93917
H      2.01094     0.69742     2.29410
H      0.28886     1.20046     2.03270
H      0.67282     2.16392    -0.30824
H      1.45060     1.26481    -1.61191
H      2.17433    -2.00252     0.62827
H      3.30171    -0.67101     0.49352
H      1.84507    -1.99224    -1.89061
H      3.67262     1.49730    -0.48508
H      3.90728    -1.59498    -3.09446
H      4.66241    -0.79862    -1.60178
H      3.96858     3.58369     0.70481
H      2.13336     3.81616     0.81543
45
bora-aza-Cope_TS-cis-6-conf17 E=-743.024941516 G=-742.710076 Imag-freq=1
C     -1.67219    -2.58802    -0.19290
C     -0.37624    -1.91560     0.03003
N     -0.16757    -0.65358    -0.43993
C     -1.38337     0.13499    -0.78616
C     -2.32801    -0.71576    -1.65271
C     -2.58485    -2.05390    -1.01699
C     -0.17446    -1.80683     2.07531
C     -2.12125     0.71913     0.45125
C     -3.16078     1.74303     0.08004
C     -4.45171     1.69453     0.42675
C      1.09187    -1.21089     2.08013
C      1.33167     0.10734     1.63348
B      1.20841    -0.01963    -0.25336
C      1.42416     1.50481    -0.83594
C      2.43473    -0.98163    -0.80649
C      3.80864    -0.69169    -0.28214
C      0.79731     2.69768    -0.17654
C      4.82812    -0.15046    -0.96582
C      1.44470     3.62686     0.54296
H     -1.81091    -3.56089     0.26857
H      0.47058    -2.58455    -0.06123
H     -1.03519     0.97242    -1.39309
H     -1.89376    -0.86046    -2.65308
H     -3.26548    -0.17060    -1.80177
H     -3.49972    -2.59086    -1.25493
H     -0.26632    -2.84087     2.39874
H     -1.05155    -1.19360     2.25603
H     -1.37784     1.19616     1.09884
H     -2.58844    -0.08382     1.03003
H     -2.80888     2.59097    -0.51057
H     -5.14655     2.47892     0.13968
H     -4.85449     0.87023     1.01186
H      1.94992    -1.87994     2.15935
H      2.33959     0.49731     1.77368
H      0.56751     0.84859     1.85705
H      1.10862     1.47557    -1.89282
H      2.50994     1.66217    -0.85445
H      2.44238    -0.87259    -1.90234
H      2.22423    -2.04115    -0.60733
H      3.98485    -0.94486     0.76561
H     -0.27959     2.82356    -0.29277
H      5.79146     0.03866    -0.49894
H      4.72933     0.12152    -2.01539
H      0.91979     4.46085     1.00171
H      2.52136     3.57897     0.69815
45
bora-aza-Cope_TS-cis-6-conf18 E=-743.025064696 G=-742.709589 Imag-freq=1
C     -0.90260    -2.77859    -0.50481
C      0.19856    -1.82737    -0.25122
N      0.03644    -0.50190    -0.52423
C     -1.36534    -0.01864    -0.67610
C     -2.14155    -0.96096    -1.61202
C     -1.99440    -2.39399    -1.18118
C      0.56340    -1.96175     1.76842
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C     -2.10308     0.18038     0.67673
C     -3.41087     0.90855     0.52351
C     -4.60008     0.46034     0.94156
C      1.62728    -1.05313     1.80144
C      1.47188     0.33082     1.57127
B      1.21655     0.43953    -0.31216
C      0.97696     2.02768    -0.66701
C      2.59872    -0.08577    -1.04850
C      3.88968     0.47772    -0.53357
C      0.10222     2.91305     0.17352
C      4.92596    -0.22660    -0.05414
C     -0.92200     3.66389    -0.25656
H     -0.74894    -3.80783    -0.19516
H      1.17361    -2.22988    -0.49646
H     -1.29643     0.95859    -1.15459
H     -1.77891    -0.84853    -2.64473
H     -3.19563    -0.66601    -1.62422
H     -2.76410    -3.11397    -1.44816
H      0.77320    -3.01798     1.91948
H     -0.41999    -1.64134     2.09787
H     -1.45348     0.77459     1.32785
H     -2.27265    -0.78300     1.16813
H     -3.35292     1.88587     0.04224
H     -5.50501     1.04862     0.81557
H     -4.70710    -0.50791     1.42677
H      2.63391    -1.46300     1.71281
H      2.35874     0.94872     1.71193
H      0.56570     0.78764     1.96335
H      0.65545     2.09647    -1.71853
H      1.98209     2.47560    -0.64443
H      2.48606     0.22268    -2.10271
H      2.68884    -1.17846    -1.06361
H      3.98315     1.56571    -0.54424
H      0.35540     2.96709     1.23406
H      5.82369     0.26070     0.31790
H      4.90818    -1.31479    -0.01877
H     -1.49298     4.29237     0.42209
H     -1.22601     3.67000    -1.30226
45
bora-aza-Cope_TS-cis-6-conf19 E=-743.026158858 G=-742.711139 Imag-freq=1
C     -0.83398    -2.73247    -0.56853
C      0.20565    -1.87204     0.03096
N      0.20922    -0.53134    -0.21198
C     -1.05756     0.06027    -0.72796
C     -1.59724    -0.79576    -1.88661
C     -1.66507    -2.24807    -1.50253
C     -0.04281    -2.08144     2.06587
C     -2.13387     0.27990     0.37078
C     -3.28603     1.12137    -0.10749
C     -4.57396     0.76107    -0.07368
C      1.02467    -1.26342     2.45449
C      1.04860     0.13303     2.24744
B      1.34108     0.30757     0.35843
C      1.33044     1.91663     0.02878
C      2.84433    -0.31575     0.09310
C      3.26321    -0.25287    -1.34665
C      0.32762     2.84706     0.64808
C      4.27704     0.46384    -1.85479
C     -0.48915     3.68806    -0.00287
H     -0.83742    -3.77929    -0.28064
H      1.18523    -2.33413     0.05345
H     -0.79143     1.04188    -1.12102
H     -0.95481    -0.67990    -2.77225
H     -2.58572    -0.42485    -2.17566
H     -2.37094    -2.90149    -2.00935
H      0.03696    -3.15396     2.22625
H     -1.05442    -1.69027     2.10420
H     -1.65624     0.79660     1.20980
H     -2.50753    -0.67985     0.74187
H     -3.02159     2.10611    -0.49540
H     -5.35943     1.42764    -0.41941
H     -4.88530    -0.21084     0.30428
H      1.97463    -1.75798     2.65889
H      1.89784     0.67464     2.66453
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H      0.10489     0.65802     2.37759
H      1.31601     2.05017    -1.06343
H      2.32578     2.26477     0.34768
H      2.90878    -1.36125     0.42535
H      3.56734     0.23892     0.70700
H      2.65879    -0.84178    -2.04085
H      0.28967     2.85364     1.73908
H      4.49615     0.46854    -2.91970
H      4.91833     1.07229    -1.21908
H     -1.17646     4.34152     0.52841
H     -0.50044     3.74596    -1.09029
45
bora-aza-Cope_TS-cis-6-conf1 E=-743.025466966 G=-742.710771 Imag-freq=1
C      1.51311    -2.06252     1.33968
C      0.39613    -1.70948     0.44418
N      0.09048    -0.40707     0.20144
C      1.14417     0.60143     0.51526
C      1.74242     0.32513     1.90528
C      2.13631    -1.11765     2.05846
C      0.96041    -2.51039    -1.40243
C      2.24757     0.71211    -0.57288
C      3.08459     1.95404    -0.41845
C      4.41506     1.97808    -0.28336
C     -0.21263    -2.16490    -2.07888
C     -0.59179    -0.83745    -2.37071
B     -1.12301    -0.09145    -0.65735
C     -1.34725     1.48157    -1.05337
C     -2.48891    -0.90732    -0.23678
C     -2.87549    -0.81311     1.21405
C     -1.94600     2.38268    -0.00801
C     -4.05351    -0.40680     1.70819
C     -3.05065     3.12860    -0.15341
H      1.75234    -3.11643     1.44185
H     -0.45674    -2.37346     0.51880
H      0.63558     1.56469     0.55719
H      1.01616     0.58975     2.68804
H      2.60555     0.98123     2.05683
H      2.90348    -1.38546     2.78058
H      1.14785    -3.55783    -1.17952
H      1.85081    -1.90216    -1.52258
H      1.75923     0.74430    -1.55304
H      2.89247    -0.17252    -0.55832
H      2.53896     2.89932    -0.43169
H      4.96004     2.91368    -0.19301
H      5.00264     1.06242    -0.26272
H     -0.98975    -2.92841    -2.12681
H     -1.49993    -0.71062    -2.95940
H      0.19907    -0.14579    -2.65516
H     -1.99491     1.51254    -1.94029
H     -0.38906     1.91716    -1.37717
H     -2.38070    -1.97519    -0.47738
H     -3.32242    -0.55016    -0.85768
H     -2.11123    -1.12409     1.92973
H     -1.42659     2.43317     0.95158
H     -4.24368    -0.37834     2.77833
H     -4.86203    -0.07747     1.05771
H     -3.42621     3.75603     0.65108
H     -3.62052     3.12628    -1.08124
45
bora-aza-Cope_TS-cis-6-conf20 E=-743.021996971 G=-742.707083 Imag-freq=1
C      1.45835    -2.06549     1.27825
C      0.32354    -1.69751     0.41336
N      0.02678    -0.39378     0.17950
C      1.09430     0.60764     0.47014
C      1.73622     0.31899     1.83868
C      2.11499    -1.12929     1.97855
C      0.85452    -2.49458    -1.46060
C      2.16502     0.72442    -0.64942
C      3.00945     1.96316    -0.51038
C      4.34365     1.98352    -0.41852
C     -0.32604    -2.13274    -2.11323
C     -0.70257    -0.80049    -2.38482
B     -1.20833    -0.06979    -0.64013
C     -1.44622     1.50707    -1.02399
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C     -2.56951    -0.88858    -0.24790
C     -3.09401    -0.88925     1.17170
C     -2.06331     2.38007     0.03201
C     -2.52697    -0.38974     2.27789
C     -3.24014     3.01638    -0.06212
H      1.68689    -3.12240     1.37383
H     -0.53653    -2.35083     0.49890
H      0.59029     1.57244     0.53551
H      1.04432     0.59398     2.64825
H      2.61372     0.96238     1.95953
H      2.89904    -1.40740     2.67832
H      1.03711    -3.54518    -1.24896
H      1.74729    -1.89062    -1.58377
H      1.64848     0.76563    -1.61441
H      2.80761    -0.16199    -0.66062
H      2.46578     2.90961    -0.49752
H      4.89326     2.91730    -0.33783
H      4.92967     1.06665    -0.42511
H     -1.10861    -2.89080    -2.15766
H     -1.62042    -0.66126    -2.95507
H      0.08549    -0.10687    -2.67110
H     -2.09794     1.53086    -1.90803
H     -0.49654     1.96192    -1.34446
H     -2.51489    -1.94670    -0.54794
H     -3.37785    -0.49440    -0.88655
H     -4.06087    -1.38588     1.29496
H     -1.49887     2.49857     0.95932
H     -3.01770    -0.47377     3.24471
H     -1.56752     0.11694     2.25699
H     -3.62841     3.62305     0.75214
H     -3.85622     2.94270    -0.95691
45
bora-aza-Cope_TS-cis-6-conf21 E=-743.027182858 G=-742.712431 Imag-freq=1
C      1.13931    -2.06179     1.61834
C      0.07731    -1.69755     0.66203
N     -0.05777    -0.41161     0.24002
C      1.11502     0.49021     0.43364
C      1.66886     0.33302     1.86010
C      1.87574    -1.11322     2.21486
C      0.53424    -2.80480    -1.04524
C      2.22707     0.30920    -0.63607
C      3.22160     1.43957    -0.62857
C      4.54344     1.30618    -0.47327
C     -0.57150    -2.39913    -1.79869
C     -0.75960    -1.08395    -2.27377
B     -1.20802    -0.06005    -0.68435
C     -1.23952     1.47015    -1.27289
C     -2.67442    -0.64538    -0.21953
C     -3.16087    -0.18432     1.12608
C     -1.63254     2.55665    -0.31050
C     -4.31661     0.44413     1.38589
C     -0.91667     3.65245    -0.01365
H      1.24298    -3.11350     1.86667
H     -0.85372    -2.23040     0.81408
H      0.72714     1.50365     0.33522
H      0.97910     0.79137     2.58452
H      2.60795     0.88999     1.94051
H      2.60141    -1.37467     2.98101
H      0.57289    -3.82897    -0.68237
H      1.50169    -2.34583    -1.22027
H      1.75089     0.27667    -1.62204
H      2.74948    -0.64255    -0.49415
H      2.80684     2.43847    -0.77450
H      5.20767     2.16577    -0.49534
H      5.00449     0.33202    -0.32288
H     -1.44578    -3.05020    -1.77111
H     -1.63306    -0.91373    -2.90271
H      0.12290    -0.54920    -2.61915
H     -1.99323     1.44809    -2.07567
H     -0.29352     1.74415    -1.76016
H     -2.65154    -1.74466    -0.20083
H     -3.41973    -0.38186    -0.98323
H     -2.49672    -0.39298     1.96799
H     -2.59112     2.42286     0.18950
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H     -4.58884     0.74483     2.39457
H     -5.02430     0.68558     0.59425
H     -1.27362     4.38892     0.70205
H      0.04906     3.84920    -0.47696
45
bora-aza-Cope_TS-cis-6-conf22 E=-743.028080851 G=-742.713110 Imag-freq=1
C     -1.65551    -2.02080    -1.48660
C     -0.39912    -1.58305    -0.84795
N     -0.22227    -0.28009    -0.49332
C     -1.45304     0.55746    -0.38899
C     -2.34743     0.33877    -1.62137
C     -2.56819    -1.12419    -1.88653
C     -0.32215    -2.67011     0.91368
C     -2.24024     0.35431     0.93496
C     -3.27034     1.42833     1.16369
C     -4.57414     1.21768     1.37520
C      0.91263    -2.17946     1.35020
C      1.12614    -0.84534     1.75795
B      1.11180     0.13822     0.11531
C      1.21104     1.69687     0.61509
C      2.41532    -0.35072    -0.76123
C      3.74902    -0.13703    -0.11130
C      1.39088     2.70238    -0.48846
C      4.63664    -1.09019     0.21056
C      2.44185     3.51834    -0.65627
H     -1.76701    -3.08299    -1.68154
H      0.48194    -2.07365    -1.24294
H     -1.11610     1.59386    -0.40478
H     -1.88936     0.80530    -2.50618
H     -3.30082     0.85342    -1.46456
H     -3.45403    -1.43887    -2.43252
H     -0.38609    -3.70250     0.57861
H     -1.23700    -2.27195     1.34092
H     -1.52533     0.38122     1.76446
H     -2.72111    -0.62913     0.95073
H     -2.89569     2.45365     1.16498
H     -5.26098     2.04067     1.55261
H     -4.99606     0.21465     1.38187
H      1.79445    -2.76731     1.09290
H      2.11768    -0.61110     2.14302
H      0.32510    -0.36357     2.31574
H      2.05485     1.78659     1.31153
H      0.31751     1.96261     1.19914
H      2.38293     0.25124    -1.68478
H      2.34892    -1.39959    -1.07429
H      4.00558     0.89623     0.12746
H      0.59171     2.75564    -1.23146
H      5.57855    -0.85162     0.69815
H      4.44780    -2.14117    -0.00312
H      2.50163     4.20561    -1.49640
H      3.27759     3.52276     0.04144
45
bora-aza-Cope_TS-cis-6-conf23 E=-743.021126951 G=-742.705315 Imag-freq=1
C      1.60626    -1.07221     1.98954
C      0.58035    -1.23447     0.94310
N      0.04055    -0.14665     0.33203
C      0.73605     1.16681     0.47867
C      1.22288     1.36319     1.92751
C      1.90060     0.14015     2.47858
C      1.54684    -2.30891    -0.54854
C      1.83623     1.50333    -0.57278
C      3.23030     0.95960    -0.39759
C      3.97075     0.42874    -1.37764
C      0.46197    -2.40310    -1.42544
C     -0.11046    -1.29278    -2.08428
B     -1.06375    -0.35961    -0.68850
C     -1.61175     0.97003    -1.48036
C     -2.25151    -1.39962    -0.21696
C     -2.99701    -1.01333     1.02975
C     -2.47026     1.92305    -0.69605
C     -4.32138    -0.83917     1.14865
C     -2.24182     3.23361    -0.51663
H      2.05572    -1.97687     2.38719
H     -0.11422    -2.04437     1.13235
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H    -0.04585    1.90428    0.30440
H     0.36928    1.61812    2.57321
H     1.89248    2.22993    1.96621
H     2.60052    0.25091    3.30330
H     1.88436   -3.20933   -0.04010
H     2.31341   -1.56123   -0.71975
H     1.91378    2.60075   -0.53690
H     1.47196    1.26329   -1.57592
H     3.67795    1.07046    0.58904
H     4.99270    0.10305   -1.20416
H     3.57900    0.29959   -2.38476
H    -0.13269   -3.31578   -1.37684
H    -0.90407   -1.50809   -2.79973
H     0.57076   -0.51568   -2.42568
H    -2.22528    0.57102   -2.30337
H    -0.79862    1.53124   -1.96022
H    -1.82973   -2.40099   -0.04854
H    -2.96643   -1.51945   -1.04334
H    -2.38479   -0.86718    1.92275
H    -3.35527    1.49124   -0.23019
H    -4.77759   -0.55634    2.09410
H    -4.99116   -0.96605    0.29947
H    -2.91299    3.85310    0.07314
H    -1.37663    3.72944   -0.95451
45
bora-aza-Cope_TS-cis-6-conf24 E=-743.025118419 G=-742.710015 Imag-freq=1
C     1.43914   -1.95956    1.64254
C     0.21674   -1.50463    0.95350
N     0.13007   -0.23716    0.46808
C     1.41221    0.50556    0.28768
C     2.29208    0.34980    1.53993
C     2.41160   -1.09070    1.95390
C     0.07925   -2.75447   -0.70908
C     2.18471    0.12150   -1.00453
C     3.27031    1.10946   -1.33944
C     4.56217    0.81049   -1.51516
C    -1.12099   -2.23258   -1.20061
C    -1.25518   -0.93225   -1.73074
B    -1.16925    0.21881   -0.17602
C    -1.15839    1.70484   -0.84209
C    -2.51134   -0.12848    0.71568
C    -3.80917    0.31644    0.11203
C    -1.20424    2.92874    0.04703
C    -4.81382   -0.47767   -0.28825
C    -1.01138    2.99259    1.37168
H     1.47792   -3.00122    1.94609
H    -0.69896   -1.89559    1.38031
H     1.13540    1.55669    0.20272
H     1.87100    0.93430    2.37136
H     3.27887    0.77807    1.33647
H     3.27432   -1.40779    2.53453
H     0.07930   -3.75273   -0.27826
H     1.02013   -2.45032   -1.15611
H     1.47157    0.10010   -1.83560
H     2.61306   -0.88239   -0.91601
H     2.94936    2.14640   -1.45460
H     5.29167    1.57301   -1.77397
H     4.93123   -0.20772   -1.40940
H    -2.03581   -2.74383   -0.89911
H    -2.23221   -0.67167   -2.13588
H    -0.42770   -0.54959   -2.32496
H    -2.02327    1.77199   -1.51946
H    -0.29975    1.83193   -1.52209
H    -2.38376    0.39595    1.67590
H    -2.58918   -1.19567    0.95551
H    -3.92988    1.39327   -0.01991
H    -1.40262    3.87016   -0.47236
H    -5.71835   -0.07254   -0.73492
H    -4.76196   -1.56016   -0.18216
H    -1.05215    3.94152    1.90086
H    -0.80454    2.10941    1.97014
45
bora-aza-Cope_TS-cis-6-conf25 E=-743.026581545 G=-742.712177 Imag-freq=1
C     1.82356   -1.90382    1.51896
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C      0.54504    -1.60343     0.84656
N      0.24132    -0.32939     0.47645
C      1.38408     0.62811     0.39014
C      2.26020     0.51593     1.64941
C      2.62582    -0.91379     1.93525
C      0.62219    -2.70797    -0.91095
C      2.22680     0.48930    -0.90797
C      3.14976     1.65952    -1.12216
C      4.47448     1.57955    -1.28864
C     -0.63955    -2.34116    -1.38857
C     -0.96508    -1.03415    -1.81084
B     -1.11471    -0.04955    -0.16497
C     -1.36156     1.48680    -0.67805
C     -2.38818    -0.66165     0.67924
C     -3.67546    -0.83309    -0.07336
C     -1.59330     2.50002     0.41017
C     -4.81923    -0.16243     0.12799
C     -2.69520     3.24424     0.58307
H      2.04009    -2.94736     1.72569
H     -0.28836    -2.18453     1.22116
H      0.94404     1.62444     0.37863
H      1.73011     0.93839     2.51597
H      3.15833     1.12685     1.51360
H      3.52447    -1.13014     2.50747
H      0.77526    -3.72690    -0.56402
H      1.50685    -2.22437    -1.31228
H      1.53866     0.43550    -1.75823
H      2.80489    -0.44031    -0.89633
H      2.67322     2.64108    -1.15322
H      5.08010     2.46552    -1.45836
H      4.99565     0.62459    -1.26445
H     -1.46665    -3.01440    -1.15887
H     -1.95036    -0.89290    -2.25225
H     -0.18893    -0.47727    -2.33177
H     -2.23453     1.48584    -1.34368
H     -0.51343     1.81897    -1.29596
H     -2.56327     0.01116     1.53172
H     -2.13364    -1.63974     1.11108
H     -3.67180    -1.58996    -0.86063
H     -0.78538     2.63215     1.13349
H     -5.70475    -0.35469    -0.47274
H     -4.90322     0.60364     0.89620
H     -2.78342     3.94782     1.40719
H     -3.54599     3.16824    -0.09134
45
bora-aza-Cope_TS-cis-6-conf26 E=-743.025466971 G=-742.710767 Imag-freq=1
C     -1.51307    -2.06258    -1.33957
C     -0.39611    -1.70948    -0.44405
N     -0.09049    -0.40705    -0.20138
C     -1.14422     0.60139    -0.51520
C     -1.74237     0.32507    -1.90526
C     -2.13622    -1.11773    -2.05842
C     -0.96041    -2.51018     1.40262
C     -2.24772     0.71191     0.57286
C     -3.08457     1.95399     0.41868
C     -4.41496     1.97819     0.28288
C      0.21262    -2.16466     2.07907
C      0.59186    -0.83721     2.37075
B      1.12301    -0.09140     0.65735
C      1.34725     1.48163     1.05334
C      2.48893    -0.90726     0.23678
C      2.87536    -0.81335    -1.21412
C      1.94603     2.38271     0.00798
C      4.05324    -0.40688    -1.70846
C      3.05084     3.12841     0.15329
H     -1.75228    -3.11649    -1.44170
H      0.45676    -2.37346    -0.51858
H     -0.63572     1.56470    -0.55705
H     -1.01605     0.58966    -2.68797
H     -2.60549     0.98115    -2.05689
H     -2.90335    -1.38558    -2.78057
H     -1.14788    -3.55764     1.17982
H     -1.85079    -1.90192     1.52269
H     -1.75949     0.74373     1.55309
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H    -2.89272    -0.17263     0.55797
H    -2.53889     2.89922     0.43272
H    -4.95983     2.91388     0.19272
H    -5.00260     1.06258     0.26144
H     0.98970    -2.92820     2.12713
H     1.49999    -0.71042     2.95946
H    -0.19894    -0.14548     2.65521
H     1.99487     1.51261     1.94028
H     0.38904     1.91722     1.37710
H     2.38084    -1.97508     0.47764
H     3.32248    -0.54987     0.85750
H     2.11112    -1.12471    -1.92965
H     1.42650     2.43338    -0.95154
H     4.24331    -0.37866    -2.77863
H     4.86173    -0.07719    -1.05814
H     3.42642     3.75582    -0.65120
H     3.62082     3.12592     1.08105
45
bora-aza-Cope_TS-cis-6-conf27 E=-743.025466968 G=-742.710766 Imag-freq=1
C    -1.51303     2.06262     1.33961
C    -0.39607     1.70954     0.44410
N    -0.09048     0.40710     0.20137
C    -1.14421    -0.60133     0.51516
C    -1.74241    -0.32505     1.90521
C    -2.13623     1.11776     2.05841
C    -0.96028     2.51037    -1.40254
C    -2.24772    -0.71191    -0.57290
C    -3.08450    -1.95402    -0.41864
C    -4.41491    -1.97831    -0.28304
C     0.21279     2.16486    -2.07894
C     0.59196     0.83741    -2.37073
B     1.12302     0.09144    -0.65736
C     1.34718    -1.48159    -1.05341
C     2.48897     0.90720    -0.23674
C     2.87534     0.81322     1.21416
C     1.94586    -2.38275    -0.00806
C     4.05314     0.40656     1.70855
C     3.05059    -3.12856    -0.15338
H    -1.75222     3.11653     1.44179
H     0.45683     2.37348     0.51871
H    -0.63568    -1.56462     0.55702
H    -1.01615    -0.58971     2.68794
H    -2.60556    -0.98112     2.05676
H    -2.90336     1.38559     2.78056
H    -1.14773     3.55782    -1.17966
H    -1.85067     1.90214    -1.52270
H    -1.75957    -0.74374    -1.55317
H    -2.89276     0.17260    -0.55802
H    -2.53874    -2.89922    -0.43243
H    -4.95972    -2.91403    -0.19282
H    -5.00262    -1.06274    -0.26184
H     0.98992     2.92837    -2.12685
H     1.50013     0.71056    -2.95935
H    -0.19891     0.14579    -2.65527
H     1.99486    -1.51257    -1.94031
H     0.38897    -1.91711    -1.37725
H     2.38095     1.97504    -0.47756
H     3.32252     0.54980    -0.85745
H     2.11113     1.12467     1.92968
H     1.42633    -2.43337     0.95146
H     4.24317     0.37829     2.77873
H     4.86161     0.07675     1.05825
H     3.42610    -3.75603     0.65111
H     3.62058    -3.12612    -1.08114
45
bora-aza-Cope_TS-cis-6-conf28 E=-743.025183556 G=-742.710421 Imag-freq=1
C    -1.97627    -2.41949    -0.27796
C    -0.64274    -1.83119    -0.04183
N    -0.36373    -0.56354    -0.45514
C    -1.53106     0.31331    -0.75957
C    -2.55304    -0.44226    -1.62656
C    -2.87490    -1.79155    -1.04892
C    -0.44841    -1.83015     2.00778
C    -2.19274     0.92944     0.50439
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C     -3.12800     2.06179     0.17395
C     -4.41800     2.12685     0.52156
C      0.85853    -1.33221     2.03234
C      1.19712    -0.01602     1.65109
B      1.04857    -0.00888    -0.24630
C      1.19264     1.57370    -0.66086
C      2.21318    -0.97677    -0.90324
C      3.56601    -1.05748    -0.25596
C      2.51571     2.21743    -0.37247
C      4.74305    -0.75059    -0.82009
C      2.72236     3.25374     0.45414
H     -2.16144    -3.40550     0.13686
H      0.16704    -2.54125    -0.16265
H     -1.14023     1.13802    -1.35655
H     -2.16149    -0.56576    -2.64731
H     -3.45831     0.16638    -1.71968
H     -3.82457    -2.26238    -1.29056
H     -0.61789    -2.86818     2.28336
H     -1.27807    -1.16178     2.21541
H     -1.39733     1.31599     1.15112
H     -2.72787     0.16028     1.07093
H     -2.69136     2.89052    -0.38650
H     -5.03328     2.98453     0.26393
H     -4.89938     1.32565     1.07882
H      1.66227    -2.06900     2.07017
H      2.23235     0.28819     1.79737
H      0.49014     0.76629     1.92257
H      0.40569     2.18621    -0.20208
H      1.02805     1.61602    -1.75187
H      2.34476    -0.65458    -1.94824
H      1.83359    -2.00747    -0.96316
H      3.58518    -1.42692     0.77126
H      3.37974     1.78935    -0.87932
H      5.67907    -0.85065    -0.27645
H      4.80671    -0.38129    -1.84244
H      3.71671     3.66018     0.62151
H      1.90258     3.72521     0.99416
45
bora-aza-Cope_TS-cis-6-conf29 E=-743.029244254 G=-742.714950 Imag-freq=1
C     -1.68033    -2.36765     0.40721
C     -0.40887    -1.64733     0.61636
N     -0.12785    -0.52456    -0.10116
C     -1.27153     0.15175    -0.77627
C     -2.14815    -0.88342    -1.50212
C     -2.49538    -2.03792    -0.60461
C     -0.48499    -1.05785     2.59263
C     -2.11091     1.05303     0.17131
C     -3.02632     1.98386    -0.57809
C     -4.35211     2.06114    -0.41855
C      0.78156    -0.46420     2.63258
C      1.11299     0.71480     1.93132
B      1.22009     0.15170     0.10387
C      1.40934     1.54295    -0.74593
C      2.51313    -0.86267     0.02654
C      2.79637    -1.35505    -1.36251
C      2.71347     2.25568    -0.54100
C      2.75218    -2.63025    -1.77799
C      2.87400     3.47380    -0.00337
H     -1.88388    -3.21164     1.05909
H      0.43816    -2.30050     0.78925
H     -0.83088     0.80114    -1.53408
H     -1.62496    -1.25955    -2.39387
H     -3.05396    -0.38847    -1.86695
H     -3.39116    -2.61951    -0.80784
H     -0.64320    -1.98806     3.13297
H     -1.36573    -0.43022     2.49942
H     -1.41870     1.65693     0.76817
H     -2.69339     0.44110     0.86803
H     -2.54300     2.64781    -1.29721
H     -4.95173     2.77043    -0.98240
H     -4.88030     1.41976     0.28415
H      1.60540    -1.08861     2.97992
H      2.10927     1.12188     2.09857
H      0.34665     1.48608     1.87515
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H      0.59255     2.24788    -0.54402
H      1.33358     1.27936    -1.81455
H      2.41857    -1.72527     0.69740
H      3.38568    -0.29892     0.38901
H      3.03921    -0.59098    -2.10417
H      3.61081     1.72197    -0.85925
H      2.94621    -2.90046    -2.81293
H      2.52012    -3.44461    -1.09350
H      3.85880     3.91674     0.12117
H      2.02352     4.06510     0.33210
45
bora-aza-Cope_TS-cis-6-conf2 E=-743.027182832 G=-742.712433 Imag-freq=1
C      1.13931    -2.06188     1.61830
C      0.07731    -1.69758     0.66200
N     -0.05778    -0.41162     0.24007
C      1.11499     0.49022     0.43380
C      1.66884     0.33292     1.86024
C      1.87573    -1.11334     2.21489
C      0.53429    -2.80474    -1.04531
C      2.22701     0.30933    -0.63595
C      3.22161     1.43965    -0.62832
C      4.54350     1.30611    -0.47356
C     -0.57140    -2.39902    -1.79879
C     -0.75948    -1.08383    -2.27379
B     -1.20799    -0.06002    -0.68434
C     -1.23946     1.47022    -1.27279
C     -2.67439    -0.64541    -0.21962
C     -3.16098    -0.18434     1.12594
C     -1.63250     2.55667    -0.31037
C     -4.31685     0.44391     1.38566
C     -0.91670     3.65252    -0.01355
H      1.24299    -3.11360     1.86655
H     -0.85371    -2.23045     0.81402
H      0.72710     1.50366     0.33547
H      0.97908     0.79122     2.58469
H      2.60793     0.88988     1.94069
H      2.60139    -1.37484     2.98102
H      0.57293    -3.82892    -0.68250
H      1.50176    -2.34576    -1.22027
H      1.75078     0.27699    -1.62190
H      2.74939    -0.64247    -0.49422
H      2.80686     2.43863    -0.77370
H      5.20777     2.16567    -0.49554
H      5.00455     0.33186    -0.32372
H     -1.44569    -3.05010    -1.77130
H     -1.63289    -0.91357    -2.90279
H      0.12305    -0.54908    -2.61907
H     -1.99314     1.44821    -2.07561
H     -0.29344     1.74423    -1.76001
H     -2.65145    -1.74468    -0.20088
H     -3.41965    -0.38195    -0.98339
H     -2.49682    -0.39283     1.96788
H     -2.59105     2.42280     0.18970
H     -4.58918     0.74462     2.39431
H     -5.02454     0.68518     0.59398
H     -1.27367     4.38897     0.70218
H      0.04899     3.84935    -0.47690
45
bora-aza-Cope_TS-cis-6-conf30 E=-743.029015823 G=-742.714602 Imag-freq=1
C     -1.89988    -2.36427     0.11743
C     -0.59971    -1.74933     0.44862
N     -0.21455    -0.58745    -0.14825
C     -1.28166     0.21966    -0.80605
C     -2.18247    -0.68619    -1.66333
C     -2.64199    -1.89310    -0.89454
C     -0.73803    -1.33640     2.46892
C     -2.11088     1.08222     0.18549
C     -2.93218     2.13411    -0.51111
C     -4.25714     2.28054    -0.40080
C      0.56038    -0.83703     2.61740
C      1.00040     0.37615     2.04545
B      1.15949    -0.01374     0.18096
C      1.46567     1.43562    -0.52222
C      2.39153    -1.09416     0.04859
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C      2.66870    -1.49619    -1.37144
C      2.78705     2.05334    -0.17434
C      3.80257    -1.28707    -2.05697
C      2.97305     3.20911     0.48055
H     -2.18541    -3.24892     0.67822
H      0.19491    -2.47023     0.60021
H     -0.76590     0.90570    -1.47933
H     -1.64065    -1.01187    -2.56373
H     -3.03816    -0.10263    -2.01799
H     -3.55942    -2.39560    -1.19076
H     -0.98200    -2.29913     2.91150
H     -1.57120    -0.64460     2.39497
H     -1.41395     1.58336     0.86611
H     -2.76221     0.44746     0.79538
H     -2.37656     2.82891    -1.14364
H     -4.78606     3.07506    -0.91996
H     -4.85519     1.61249     0.21581
H      1.32461    -1.54552     2.93900
H      2.01099     0.69713     2.29405
H      0.28896     1.20036     2.03279
H      0.67282     2.16393    -0.30815
H      1.45060     1.26490    -1.61187
H      2.17428    -2.00257     0.62816
H      3.30167    -0.67106     0.49357
H      1.84522    -1.99219    -1.89072
H      3.67262     1.49729    -0.48504
H      3.90750    -1.59478    -3.09442
H      4.66249    -0.79846    -1.60166
H      3.96861     3.58361     0.70495
H      2.13340     3.81611     0.81559
45
bora-aza-Cope_TS-cis-6-conf31 E=-743.028624186 G=-742.713818 Imag-freq=1
C      1.30569    -2.21839     1.47639
C      0.10401    -1.63354     0.84982
N      0.08565    -0.32045     0.48932
C      1.40528     0.36433     0.36762
C      2.28273     0.03996     1.58881
C      2.32618    -1.43799     1.85922
C     -0.12613    -2.70855    -0.90143
C      2.14483     0.06651    -0.96593
C      3.28895     1.01300    -1.21415
C      4.55823     0.65277    -1.43413
C     -1.29856    -2.07519    -1.32719
C     -1.35509    -0.72719    -1.73989
B     -1.18864     0.26224    -0.10367
C     -1.09726     1.81551    -0.62060
C     -2.53467    -0.05774     0.79103
C     -3.83655     0.38489     0.19247
C     -1.12089     2.85098     0.46865
C     -4.85773    -0.41008    -0.16067
C     -0.19881     3.79991     0.69124
H      1.28957    -3.28537     1.67639
H     -0.82558    -2.00859     1.26067
H      1.18779     1.43177     0.39009
H      1.89772     0.56251     2.47731
H      3.29016     0.43288     1.41766
H      3.17414    -1.85684     2.39545
H     -0.18281    -3.74013    -0.56247
H      0.82445    -2.42548    -1.34222
H      1.42604     0.17411    -1.78555
H      2.50841    -0.96623    -0.98456
H      3.03399     2.07430    -1.22213
H      5.33323     1.39009    -1.62474
H      4.86250    -0.39203    -1.43436
H     -2.24084    -2.55259    -1.05596
H     -2.31684    -0.37457    -2.11042
H     -0.51006    -0.34808    -2.31164
H     -1.98223     1.97236    -1.25580
H     -0.23159     1.99013    -1.27288
H     -2.39186     0.47841     1.74434
H     -2.62093    -1.11948     1.05103
H     -3.95047     1.45702     0.02096
H     -1.97633     2.81269     1.14574
H     -5.76444    -0.00975    -0.60704
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H     -4.81751    -1.48838    -0.01488
H     -0.29258     4.50258     1.51533
H      0.67858     3.90568     0.05528
45
bora-aza-Cope_TS-cis-6-conf32 E=-743.029015812 G=-742.714604 Imag-freq=1
C     -1.90000    -2.36415     0.11758
C     -0.59975    -1.74930     0.44866
N     -0.21455    -0.58745    -0.14820
C     -1.28161     0.21968    -0.80605
C     -2.18240    -0.68620    -1.66331
C     -2.64208    -1.89298    -0.89441
C     -0.73791    -1.33638     2.46896
C     -2.11082     1.08234     0.18543
C     -2.93232     2.13400    -0.51129
C     -4.25728     2.28031    -0.40080
C      0.56048    -0.83695     2.61737
C      1.00047     0.37628     2.04544
B      1.15955    -0.01383     0.18107
C      1.46583     1.43548    -0.52215
C      2.39148    -1.09437     0.04849
C      2.66863    -1.49612    -1.37163
C      2.78711     2.05328    -0.17406
C      3.80259    -1.28713    -2.05705
C      2.97292     3.20935     0.48038
H     -2.18561    -3.24871     0.67846
H      0.19482    -2.47026     0.60019
H     -0.76580     0.90567    -1.47935
H     -1.64049    -1.01203    -2.56359
H     -3.03801    -0.10263    -2.01816
H     -3.55959    -2.39539    -1.19055
H     -0.98182    -2.29911     2.91158
H     -1.57111    -0.64461     2.39507
H     -1.41388     1.58368     0.86589
H     -2.76203     0.44763     0.79549
H     -2.37690     2.82871    -1.14409
H     -4.78638     3.07465    -0.92006
H     -4.85516     1.61234     0.21607
H      1.32475    -1.54540     2.93900
H      2.01104     0.69727     2.29412
H      0.28901     1.20047     2.03284
H      0.67292     2.16380    -0.30836
H      1.45102     1.26462    -1.61179
H      2.17412    -2.00288     0.62786
H      3.30167    -0.67148     0.49359
H      1.84505    -1.99179    -1.89106
H      3.67278     1.49707    -0.48419
H      3.90749    -1.59462    -3.09456
H      4.66261    -0.79884    -1.60158
H      3.96842     3.58391     0.70497
H      2.13317     3.81652     0.81486
45
bora-aza-Cope_TS-cis-6-conf33 E=-743.019703143 G=-742.704140 Imag-freq=1
C     -1.49674    -2.28015    -0.76435
C     -0.38877    -1.68643     0.00945
N      0.06963    -0.44180    -0.29686
C     -0.78790     0.42865    -1.15210
C     -1.36016    -0.38014    -2.33162
C     -1.93708    -1.69546    -1.88676
C     -1.07374    -1.58285     1.94339
C     -1.87930     1.27269    -0.42495
C     -3.21003     0.65289    -0.08667
C     -3.84136     0.79698     1.08466
C      0.07869    -1.03553     2.51976
C      0.55062     0.26507     2.23050
B      1.26917     0.09287     0.47109
C      1.85400     1.56824     0.04461
C      2.51883    -0.97747     0.60379
C      3.21908    -1.23431    -0.69835
C      1.10138     2.83957     0.31056
C      4.48895    -0.92393    -0.99998
C      0.78518     3.78139    -0.59004
H     -1.87640    -3.24072    -0.42969
H      0.37993    -2.40322     0.27227
H     -0.10028     1.16731    -1.56334
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H     -0.57008     -0.56676     -3.07409
H     -2.11734      0.22173     -2.84705
H     -2.69169     -2.17730     -2.50387
H     -1.33359     -2.61180      2.18260
H     -1.91652     -0.93879      1.71686
H     -2.07927      2.10501     -1.11656
H     -1.44820      1.73359      0.46684
H     -3.71498      0.10800     -0.88290
H     -4.82894      0.37624      1.25299
H     -3.39087      1.33823      1.91449
H      0.78008     -1.73144      2.98071
H      1.40939      0.61057      2.80687
H     -0.20494      1.03569      2.09217
H      2.13524      1.53539     -1.01882
H      2.80753      1.64445      0.59119
H      2.18025     -1.94127      1.00865
H      3.24000     -0.58368      1.33339
H      2.61313     -1.70590     -1.47595
H      0.81302      3.01799      1.34853
H      4.90916     -1.12685     -1.98200
H      5.14750     -0.45240     -0.27225
H      0.24735      4.68310     -0.30821
H      1.04742      3.67591     -1.64176
45
bora-aza-Cope_TS-cis-6-conf34 E=-743.025174292 G=-742.710142 Imag-freq=1
C     -1.31460     -2.67188     -0.60371
C     -0.09344     -1.92561     -0.23779
N     -0.01380     -0.58500     -0.47036
C     -1.30137      0.13032     -0.70061
C     -2.14983     -0.64377     -1.72391
C     -2.27369     -2.09211     -1.33947
C      0.09215     -2.17055      1.79434
C     -2.09604      0.41461      0.60386
C     -3.24916      1.35681      0.38735
C     -4.52490      1.10336      0.70047
C      1.28417     -1.45180      1.94273
C      1.37519     -0.05616      1.75136
B      1.28501      0.14246     -0.14803
C      1.34178      1.75367     -0.45617
C      2.61260     -0.58528     -0.81243
C      3.94287     -0.22482     -0.22290
C      0.57140      2.75343      0.35610
C      4.89516      0.52589     -0.79689
C     -0.27803      3.67987     -0.11159
H     -1.35641     -3.72024     -0.32448
H      0.81686     -2.47962     -0.43175
H     -1.03543      1.09442     -1.13462
H     -1.69732     -0.56632     -2.72385
H     -3.13694     -0.17653     -1.79788
H     -3.12923     -2.66588     -1.68722
H      0.11464     -3.25015      1.92203
H     -0.84833     -1.70018      2.06332
H     -1.40856      0.87359      1.32197
H     -2.46044     -0.51903      1.04424
H     -2.99280      2.32365     -0.04813
H     -5.30744      1.83874      0.53417
H     -4.82791      0.15350      1.13672
H      2.21163     -2.02556      1.92263
H      2.32995      0.41199      1.98969
H      0.52295      0.53235      2.08334
H      1.11592      1.90553     -1.52393
H      2.40688      2.00892     -0.34584
H      2.61185     -0.31252     -1.87950
H      2.52365     -1.67937     -0.77768
H      4.14446     -0.61192      0.77834
H      0.75297      2.73642      1.43258
H      5.82907      0.74996     -0.28762
H      4.76867      0.94066     -1.79553
H     -0.78126      4.37907      0.55135
H     -0.50143      3.76526     -1.17405
45
bora-aza-Cope_TS-cis-6-conf35 E=-743.026158853 G=-742.711139 Imag-freq=1
C     -0.83428     -2.73233     -0.56872
C      0.20547     -1.87205      0.03080
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N      0.20918    -0.53134    -0.21205
C     -1.05754     0.06043    -0.72799
C     -1.59730    -0.79546     -1.88669
C     -1.66532    -2.24778     -1.50267
C     -0.04299    -2.08157      2.06570
C     -2.13379     0.28009      0.37080
C     -3.28602     1.12148     -0.10745
C     -4.57395     0.76118     -0.07339
C      1.02459    -1.26371      2.45438
C      1.04870     0.13275      2.24742
B      1.34110     0.30744      0.35845
C      1.33062     1.91653      0.02895
C      2.84430    -0.31600      0.09308
C      3.26328    -0.25289     -1.34663
C      0.32779     2.84698      0.64818
C      4.27719     0.46384     -1.85458
C     -0.48889     3.68804     -0.00281
H     -0.83784    -3.77917     -0.28088
H      1.18499    -2.33427      0.05325
H     -0.79131     1.04205     -1.12098
H     -0.95482    -0.67965     -2.77230
H     -2.58573    -0.42442     -2.17576
H     -2.37129    -2.90108     -2.00951
H      0.03664    -3.15411      2.22601
H     -1.05454    -1.69026      2.10406
H     -1.65612     0.79689      1.20974
H     -2.50738    -0.67964      0.74199
H     -3.02165     2.10616     -0.49556
H     -5.35947     1.42769     -0.41912
H     -4.88523    -0.21067      0.30476
H      1.97449    -1.75840      2.65876
H      1.89798     0.67422      2.66462
H      0.10504     0.65784      2.37763
H      1.31639     2.05018     -1.06325
H      2.32594     2.26455      0.34805
H      2.90861    -1.36156      0.42513
H      3.56734     0.23847      0.70713
H      2.65888    -0.84166     -2.04097
H      0.28974     2.85353      1.73918
H      4.49637     0.46871     -2.91948
H      4.91847     1.07216     -1.21873
H     -1.17622     4.34150      0.52842
H     -0.50007     3.74598     -1.09024
45
bora-aza-Cope_TS-cis-6-conf36 E=-743.029244254 G=-742.714951 Imag-freq=1
C      1.68028     2.36768      0.40722
C      0.40882     1.64735      0.61633
N      0.12785     0.52456     -0.10117
C      1.27153    -0.15171     -0.77629
C      2.14811     0.88349     -1.50214
C      2.49535     2.03797     -0.60460
C      0.48489     1.05790      2.59264
C      2.11094    -1.05301      0.17124
C      3.02646    -1.98369     -0.57822
C      4.35220    -2.06114     -0.41837
C     -0.78159     0.46409      2.63257
C     -1.11292    -0.71492      1.93125
B     -1.22009    -0.15171      0.10386
C     -1.40934    -1.54296     -0.74593
C     -2.51314     0.86264      0.02659
C     -2.79645     1.35504     -1.36244
C     -2.71345    -2.25572     -0.54097
C     -2.75226     2.63024     -1.77791
C     -2.87393    -3.47390     -0.00345
H      1.88382     3.21165      1.05913
H     -0.43822     2.30050      0.78919
H      0.83089    -0.80109     -1.53411
H      1.62488     1.25965     -2.39385
H      3.05393     0.38858     -1.86703
H      3.39115     2.61956     -0.80779
H      0.64295     1.98814      3.13297
H      1.36574     0.43042      2.49947
H      1.41877    -1.65704      0.76801
H      2.69334    -0.44113      0.86806
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H      2.54326    -2.64738    -1.29765
H      4.95190    -2.77033    -0.98227
H      4.88027    -1.42000     0.28464
H     -1.60549     1.08839     2.97994
H     -2.10915    -1.12211     2.09856
H     -0.34650    -1.48612     1.87508
H     -0.59253    -2.24788    -0.54403
H     -1.33360    -1.27938    -1.81455
H     -2.41858     1.72524     0.69746
H     -3.38567     0.29887     0.38908
H     -3.03932     0.59098    -2.10410
H     -3.61082    -1.72198    -0.85909
H     -2.94634     2.90046    -2.81285
H     -2.52016     3.44460    -1.09343
H     -3.85872    -3.91685     0.12112
H     -2.02341    -4.06523     0.33190
45
bora-aza-Cope_TS-cis-6-conf37 E=-743.028080877 G=-742.713109 Imag-freq=1
C     -1.65545    -2.02100    -1.48650
C     -0.39908    -1.58315    -0.84786
N     -0.22227    -0.28016    -0.49336
C     -1.45308     0.55732    -0.38903
C     -2.34746     0.33854    -1.62140
C     -2.56817    -1.12444    -1.88647
C     -0.32213    -2.66997     0.91387
C     -2.24029     0.35414     0.93492
C     -3.27010     1.42838     1.16386
C     -4.57400     1.21804     1.37510
C      0.91264    -2.17931     1.35033
C      1.12628    -0.84512     1.75791
B      1.11178     0.13817     0.11539
C      1.21095     1.69690     0.61499
C      2.41530    -0.35068    -0.76120
C      3.74900    -0.13697    -0.11127
C      1.39074     2.70229    -0.48868
C      4.63668    -1.09010     0.21051
C      2.44157     3.51844    -0.65645
H     -1.76690    -3.08320    -1.68138
H      0.48201    -2.07376    -1.24279
H     -1.11621     1.59374    -0.40485
H     -1.88939     0.80502    -2.50623
H     -3.30087     0.85318    -1.46463
H     -3.45400    -1.43919    -2.43244
H     -0.38610    -3.70240     0.57893
H     -1.23697    -2.27174     1.34108
H     -1.52536     0.38069     1.76441
H     -2.72142    -0.62918     0.95051
H     -2.89514     2.45357     1.16555
H     -5.26062     2.04118     1.55266
H     -4.99622     0.21513     1.38137
H      1.79445    -2.76723     1.09312
H      2.11782    -0.61106     2.14310
H      0.32532    -0.36321     2.31572
H      2.05475     1.78674     1.31141
H      0.31740     1.96267     1.19901
H      2.38289     0.25131    -1.68472
H      2.34895    -1.39955    -1.07429
H      4.00552     0.89630     0.12753
H      0.59168     2.75527    -1.23182
H      5.57859    -0.85150     0.69810
H      4.44790    -2.14107    -0.00323
H      2.50133     4.20560    -1.49667
H      3.27721     3.52312     0.04138
45
bora-aza-Cope_TS-cis-6-conf38 E=-743.025466948 G=-742.710769 Imag-freq=1
C     -1.51293    -2.06256    -1.33969
C     -0.39604    -1.70945    -0.44410
N     -0.09044    -0.40702    -0.20141
C     -1.14418     0.60141    -0.51526
C     -1.74228     0.32510    -1.90534
C     -2.13610    -1.11771    -2.05852
C     -0.96048    -2.51017     1.40252
C     -2.24768     0.71191     0.57280
C     -3.08463     1.95391     0.41857
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C     -4.41505     1.97803     0.28304
C      0.21248    -2.16463     2.07907
C      0.59169    -0.83715     2.37076
B      1.12303    -0.09141     0.65742
C      1.34727     1.48162     1.05338
C      2.48894    -0.90730     0.23691
C      2.87546    -0.81340    -1.21396
C      1.94593     2.38272     0.00796
C      4.05336    -0.40687    -1.70823
C      3.05068     3.12851     0.15318
H     -1.75212    -3.11647    -1.44186
H      0.45686    -2.37341    -0.51856
H     -0.63568     1.56472    -0.55707
H     -1.01593     0.58970    -2.68801
H     -2.60540     0.98118    -2.05700
H     -2.90321    -1.38556    -2.78070
H     -1.14792    -3.55762     1.17969
H     -1.85088    -1.90191     1.52252
H     -1.75944     0.74382     1.55302
H     -2.89262    -0.17268     0.55796
H     -2.53899     2.89918     0.43235
H     -4.95998     2.91367     0.19285
H     -5.00264     1.06238     0.26187
H      0.98956    -2.92817     2.12722
H      1.49971    -0.71035     2.95964
H     -0.19919    -0.14545     2.65507
H      1.99499     1.51262     1.94025
H      0.38909     1.91719     1.37725
H      2.38079    -1.97513     0.47775
H      3.32247    -0.54996     0.85768
H      2.11129    -1.12480    -1.92954
H      1.42635     2.43330    -0.95154
H      4.24350    -0.37866    -2.77839
H      4.86179    -0.07714    -1.05786
H      3.42617     3.75592    -0.65135
H      3.62071     3.12610     1.08092
45
bora-aza-Cope_TS-cis-6-conf39 E=-743.027656662 G=-742.712492 Imag-freq=1
C      1.22018    -2.27680     1.03252
C      0.15389    -1.68580     0.20118
N      0.00753    -0.33515     0.12875
C      1.16904     0.49681     0.55433
C      1.72992    -0.02265     1.88946
C      1.95092    -1.50943     1.85367
C      0.62599    -2.30263    -1.72283
C      2.27922     0.62198    -0.52546
C      3.25425     1.72875    -0.22341
C      4.57931     1.58394    -0.11260
C     -0.49143    -1.74033    -2.34782
C     -0.71054    -0.35174    -2.46742
B     -1.15758     0.21582    -0.66902
C     -1.22388     1.84558    -0.83832
C     -2.61567    -0.48466    -0.34964
C     -2.98328    -0.50565     1.10570
C     -1.74822     2.61584     0.34099
C     -3.22749    -1.60005     1.84336
C     -2.87306     3.34567     0.36996
H      1.33394    -3.35595     0.99929
H     -0.77633    -2.24117     0.21360
H      0.77449     1.49853     0.72647
H      1.03871     0.22277     2.70932
H      2.66403     0.50349     2.11106
H      2.68140    -1.95398     2.52497
H      0.68734    -3.38487    -1.63826
H      1.58350    -1.79508    -1.77642
H      1.79850     0.83844    -1.48588
H      2.81739    -0.32512    -0.63593
H      2.82109     2.72313    -0.10051
H      5.22825     2.43146     0.09022
H      5.05840     0.61343    -0.22524
H     -1.35237    -2.39491    -2.48583
H     -1.59404    -0.04602    -3.02719
H      0.15713     0.27421    -2.66755
H     -1.86763     2.05924    -1.70229
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H    -0.22957    2.23655   -1.10208
H    -2.69887   -1.50354   -0.74755
H    -3.36327    0.11350   -0.89400
H    -3.03128    0.46491    1.60059
H    -1.15960    2.56116    1.25971
H    -3.46547   -1.53337    2.90215
H    -3.19984   -2.59895    1.41016
H    -3.19577    3.86162    1.27072
H    -3.50966    3.44451   -0.50777
45
bora-aza-Cope_TS-cis-6-conf3 E=-743.026158859 G=-742.711139 Imag-freq=1
C    -0.83402   -2.73244   -0.56859
C     0.20563   -1.87204    0.03090
N     0.20921   -0.53133   -0.21198
C    -1.05757    0.06030   -0.72794
C    -1.59724   -0.79568   -1.88662
C    -1.66511   -2.24801   -1.50257
C    -0.04279   -2.08153    2.06584
C    -2.13388    0.27988    0.37081
C    -3.28603    1.12139   -0.10744
C    -4.57396    0.76109   -0.07371
C     1.02470   -1.26352    2.45446
C     1.04863    0.13294    2.24746
B     1.34109    0.30756    0.35843
C     1.33045    1.91662    0.02884
C     2.84433   -0.31577    0.09306
C     3.26319   -0.25280   -1.34669
C     0.32760    2.84702    0.64815
C     4.27707    0.46389   -1.85479
C    -0.48913    3.68806   -0.00279
H    -0.83749   -3.77927   -0.28071
H     1.18521   -2.33415    0.05336
H    -0.79144    1.04193   -1.12095
H    -0.95478   -0.67982   -2.77223
H    -2.58570   -0.42475   -2.17569
H    -2.37101   -2.90139   -2.00939
H     0.03699   -3.15405    2.22617
H    -1.05440   -1.69036    2.10420
H    -1.65626    0.79654    1.20986
H    -2.50756   -0.67987    0.74184
H    -3.02157    2.10617   -0.49525
H    -5.35942    1.42768   -0.41942
H    -4.88531   -0.21085    0.30415
H     1.97467   -1.75808    2.65882
H     1.89787    0.67454    2.66454
H     0.10492    0.65793    2.37763
H     1.31605    2.05021   -1.06336
H     2.32578    2.26477    0.34777
H     2.90877   -1.36129    0.42523
H     3.56736    0.23884    0.70698
H     2.65873   -0.84162   -2.04093
H     0.28961    2.85354    1.73915
H     4.49617    0.46866   -2.91970
H     4.91840    1.07225   -1.21904
H    -1.17646    4.34149    0.52849
H    -0.50037    3.74602   -1.09021
45
bora-aza-Cope_TS-cis-6-conf4 E=-743.029015822 G=-742.714602 Imag-freq=1
C    -1.89988   -2.36427    0.11753
C    -0.59972   -1.74930    0.44872
N    -0.21455   -0.58747   -0.14824
C    -1.28166    0.21959   -0.80609
C    -2.18242   -0.68631   -1.66336
C    -2.64195   -1.89318   -0.89452
C    -0.73809   -1.33619    2.46898
C    -2.11090    1.08214    0.18544
C    -2.93210    2.13413   -0.51115
C    -4.25705    2.28065   -0.40089
C     0.56032   -0.83679    2.61750
C     1.00041    0.37633    2.04546
B     1.15948   -0.01371    0.18097
C     1.46567    1.43559   -0.52230
C     2.39152   -1.09415    0.04869
C     2.66862   -1.49631   -1.37132
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C      2.78707     2.05330    -0.17451
C      3.80247    -1.28727    -2.05692
C      2.97312     3.20907     0.48038
H     -2.18543    -3.24887     0.67837
H      0.19488    -2.47021     0.60037
H     -0.76590     0.90565    -1.47936
H     -1.64059    -1.01201    -2.56373
H     -3.03812    -0.10278    -2.01806
H     -3.55935    -2.39573    -1.19075
H     -0.98205    -2.29888     2.91166
H     -1.57126    -0.64441     2.39493
H     -1.41398     1.58317     0.86614
H     -2.76233     0.44738     0.79523
H     -2.37640     2.82891    -1.14362
H     -4.78589     3.07524    -0.92003
H     -4.85518     1.61261     0.21566
H      1.32452    -1.54525     2.93925
H      2.01098     0.69731     2.29412
H      0.28897     1.20053     2.03266
H      0.67284     2.16393    -0.30826
H      1.45056     1.26480    -1.61195
H      2.17429    -2.00250     0.62837
H      3.30168    -0.67100     0.49359
H      1.84512    -1.99236    -1.89051
H      3.67262     1.49726    -0.48528
H      3.90734    -1.59508    -3.09434
H      4.66242    -0.79863    -1.60169
H      3.96870     3.58357     0.70472
H      2.13349     3.81607     0.81549
45
bora-aza-Cope_TS-cis-6-conf5 E=-743.028624188 G=-742.713819 Imag-freq=1
C      1.30570    -2.21846     1.47623
C      0.10402    -1.63351     0.84976
N      0.08569    -0.32040     0.48935
C      1.40533     0.36438     0.36776
C      2.28271     0.03987     1.58895
C      2.32621    -1.43812     1.85913
C     -0.12627    -2.70841    -0.90157
C      2.14482     0.06667    -0.96584
C      3.28919     1.01290    -1.21390
C      4.55833     0.65234    -1.43418
C     -1.29869    -2.07496    -1.32723
C     -1.35516    -0.72695    -1.73990
B     -1.18858     0.26232    -0.10366
C     -1.09718     1.81558    -0.62063
C     -2.53464    -0.05765     0.79100
C     -3.83655     0.38466     0.19225
C     -1.12091     2.85110     0.46858
C     -4.85778    -0.41050    -0.16033
C     -0.19890     3.80010     0.69114
H      1.28959    -3.28546     1.67606
H     -0.82558    -2.00855     1.26061
H      1.18787     1.43183     0.39030
H      1.89755     0.56224     2.47751
H      3.29013     0.43291     1.41798
H      3.17421    -1.85705     2.39523
H     -0.18298    -3.73999    -0.56264
H      0.82429    -2.42536    -1.34240
H      1.42595     0.17471    -1.78534
H      2.50808    -0.96617    -0.98475
H      3.03456     2.07427    -1.22148
H      5.33353     1.38948    -1.62466
H      4.86226    -0.39256    -1.43481
H     -2.24098    -2.55228    -1.05592
H     -2.31691    -0.37426    -2.11038
H     -0.51016    -0.34794    -2.31176
H     -1.98209     1.97240    -1.25591
H     -0.23146     1.99019    -1.27284
H     -2.39198     0.47876     1.74419
H     -2.62079    -1.11932     1.05127
H     -3.95046     1.45669     0.02011
H     -1.97638     2.81279     1.14563
H     -5.76452    -0.01042    -0.60687
H     -4.81756    -1.48872    -0.01391
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H     -0.29275     4.50282     1.51517
H      0.67851     3.90590     0.05520
45
bora-aza-Cope_TS-cis-6-conf6 E=-743.026581546 G=-742.712176 Imag-freq=1
C      1.82355    -1.90378     1.51900
C      0.54504    -1.60342     0.84656
N      0.24132    -0.32938     0.47645
C      1.38406     0.62813     0.39015
C      2.26018     0.51596     1.64942
C      2.62580    -0.91375     1.93530
C      0.62224    -2.70795    -0.91090
C      2.22676     0.48934    -0.90797
C      3.14978     1.65951    -1.12214
C      4.47449     1.57948    -1.28869
C     -0.63950    -2.34116    -1.38858
C     -0.96503    -1.03416    -1.81084
B     -1.11472    -0.04958    -0.16499
C     -1.36160     1.48677    -0.67806
C     -2.38818    -0.66172     0.67919
C     -3.67547    -0.83307    -0.07340
C     -1.59332     2.49999     0.41018
C     -4.81925    -0.16244     0.12803
C     -2.69517     3.24428     0.58304
H      2.04008    -2.94732     1.72575
H     -0.28836    -2.18452     1.22116
H      0.94401     1.62447     0.37864
H      1.73012     0.93846     2.51598
H      3.15832     1.12687     1.51359
H      3.52442    -1.13009     2.50754
H      0.77531    -3.72688    -0.56396
H      1.50690    -2.22436    -1.31223
H      1.53858     0.43562    -1.75820
H      2.80480    -0.44030    -0.89637
H      2.67329     2.64111    -1.15313
H      5.08015     2.46543    -1.45839
H      4.99561     0.62449    -1.26457
H     -1.46660    -3.01442    -1.15892
H     -1.95028    -0.89295    -2.25232
H     -0.18887    -0.47730    -2.33178
H     -2.23459     1.48580    -1.34367
H     -0.51349     1.81896    -1.29599
H     -2.56325     0.01100     1.53174
H     -2.13366    -1.63986     1.11093
H     -3.67183    -1.58984    -0.86077
H     -0.78543     2.63204     1.13353
H     -5.70477    -0.35463    -0.47270
H     -4.90323     0.60354     0.89633
H     -2.78337     3.94785     1.40718
H     -3.54594     3.16835    -0.09140
45
bora-aza-Cope_TS-cis-6-conf7 E=-743.027656692 G=-742.712494 Imag-freq=1
C      1.22030    -2.27650     1.03288
C      0.15398    -1.68573     0.20143
N      0.00751    -0.33511     0.12875
C      1.16898     0.49699     0.55419
C      1.72977    -0.02217     1.88947
C      1.95096    -1.50892     1.85393
C      0.62615    -2.30304    -1.72251
C      2.27923     0.62195    -0.52556
C      3.25430     1.72872    -0.22360
C      4.57934     1.58386    -0.11262
C     -0.49124    -1.74080    -2.34760
C     -0.71026    -0.35221    -2.46733
B     -1.15766     0.21572    -0.66905
C     -1.22405     1.84544    -0.83858
C     -2.61568    -0.48488    -0.34971
C     -2.98349    -0.50555     1.10559
C     -1.74831     2.61587     0.34066
C     -3.22764    -1.59981     1.84349
C     -2.87312     3.34573     0.36960
H      1.33419    -3.35564     0.99980
H     -0.77621    -2.24117     0.21397
H      0.77441     1.49874     0.72608
H      1.03842     0.22329     2.70919
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H      2.66378     0.50413     2.11110
H      2.68148    -1.95330     2.52530
H      0.68741    -3.38525    -1.63769
H      1.58369    -1.79556    -1.77619
H      1.79859     0.83831    -1.48604
H      2.81737    -0.32519    -0.63587
H      2.82118     2.72315    -0.10093
H      5.22831     2.43137     0.09012
H      5.05838     0.61329    -0.22504
H     -1.35222    -2.39535    -2.48546
H     -1.59377    -0.04643    -3.02705
H      0.15746     0.27367    -2.66748
H     -1.86789     2.05895    -1.70253
H     -0.22978     2.23641    -1.10250
H     -2.69867    -1.50388    -0.74737
H     -3.36330     0.11302    -0.89433
H     -3.03169     0.46512     1.60023
H     -1.15963     2.56131     1.25936
H     -3.46577    -1.53290     2.90223
H     -3.19979    -2.59881     1.41054
H     -3.19577     3.86182     1.27031
H     -3.50977     3.44447    -0.50811
45
bora-aza-Cope_TS-cis-6-conf8 E=-743.026158856 G=-742.711139 Imag-freq=1
C     -0.83399    -2.73245    -0.56851
C      0.20563    -1.87202     0.03100
N      0.20921    -0.53132    -0.21192
C     -1.05757     0.06028    -0.72789
C     -1.59721    -0.79571    -1.88657
C     -1.66506    -2.24803    -1.50252
C     -0.04287    -2.08141     2.06593
C     -2.13395     0.27983     0.37082
C     -3.28603     1.12141    -0.10746
C     -4.57397     0.76110    -0.07392
C      1.02466    -1.26344     2.45454
C      1.04867     0.13302     2.24745
B      1.34111     0.30756     0.35848
C      1.33049     1.91661     0.02880
C      2.84434    -0.31579     0.09302
C      3.26312    -0.25290    -1.34675
C      0.32772     2.84706     0.64813
C      4.27696     0.46376    -1.85494
C     -0.48906     3.68808    -0.00279
H     -0.83744    -3.77927    -0.28063
H      1.18521    -2.33412     0.05351
H     -0.79145     1.04191    -1.12090
H     -0.95474    -0.67984    -2.77218
H     -2.58568    -0.42480    -2.17566
H     -2.37093    -2.90144    -2.00936
H      0.03685    -3.15393     2.22632
H     -1.05445    -1.69018     2.10423
H     -1.65641     0.79640     1.20998
H     -2.50768    -0.67995     0.74174
H     -3.02153     2.10623    -0.49512
H     -5.35939     1.42774    -0.41965
H     -4.88537    -0.21089     0.30379
H      1.97458    -1.75803     2.65898
H      1.89794     0.67456     2.66456
H      0.10500     0.65808     2.37760
H      1.31604     2.05016    -1.06341
H      2.32586     2.26474     0.34767
H      2.90878    -1.36130     0.42524
H      3.56740     0.23884     0.70688
H      2.65863    -0.84176    -2.04093
H      0.28980     2.85364     1.73914
H      4.49601     0.46848    -2.91987
H      4.91833     1.07217    -1.21926
H     -1.17634     4.34155     0.52851
H     -0.50038     3.74598    -1.09021
45
bora-aza-Cope_TS-cis-6-conf9 E=-743.025064702 G=-742.709587 Imag-freq=1
C     -0.90286    -2.77848    -0.50484
C      0.19842    -1.82738    -0.25134
N      0.03640    -0.50187    -0.52429
```

```
C      -1.36535     -0.01849     -0.67614
C      -2.14168     -0.96075     -1.61200
C      -1.99469     -2.39378     -1.18110
C       0.56346     -1.96194      1.76829
C      -2.10295      0.18073      0.67673
C      -3.41092      0.90858      0.52353
C      -4.60000      0.46015      0.94174
C       1.62736     -1.05335      1.80125
C       1.47194      0.33060      1.57121
B       1.21653      0.43949     -0.31229
C       0.97704      2.02767     -0.66704
C       2.59872     -0.08588     -1.04853
C       3.88968      0.47761     -0.53360
C       0.10245      2.91307      0.17361
C       4.92587     -0.22670     -0.05395
C      -0.92179      3.66397     -0.25632
H      -0.74928     -3.80774     -0.19518
H       1.17341     -2.22998     -0.49667
H      -1.29636      0.95872     -1.15468
H      -1.77901     -0.84842     -2.64472
H      -3.19572     -0.66568     -1.62423
H      -2.76450     -3.11368     -1.44798
H       0.77326     -3.01819      1.91920
H      -0.41988     -1.64154      2.09787
H      -1.45336      0.77531      1.32750
H      -2.27222     -0.78254      1.16845
H      -3.35323      1.88585      0.04213
H      -5.50507      1.04821      0.81575
H      -4.70675     -0.50806      1.42707
H       2.63398     -1.46322      1.71246
H       2.35879      0.94855      1.71167
H       0.56576      0.78735      1.96337
H       0.65542      2.09653     -1.71853
H       1.98220      2.47551     -0.64455
H       2.48609      0.22252     -2.10276
H       2.68881     -1.17857     -1.06357
H       3.98323      1.56559     -0.54448
H       0.35578      2.96709      1.23412
H       5.82360      0.26061      0.31807
H       4.90801     -1.31487     -0.01839
H      -1.49265      4.29246      0.42242
H      -1.22594      3.67010     -1.30198
```

TS_trans-2:

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45
bora-aza-Cope_TS-trans-2-conf10 E=-743.022273627 G=-742.707539 Imag-freq=1
C       2.52109      0.50181     -1.04825
C       1.03083      0.66934     -0.88340
N       0.41408     -0.25489      0.10604
C       1.22282     -0.99123      0.91120
C       2.66939     -0.59262      1.13923
C       3.29608     -0.04743     -0.11122
C       0.69308      2.15574     -0.54875
C       1.43361     -2.80439     -0.01642
C       0.08694     -3.08771     -0.25018
C      -0.71501     -2.30215     -1.11036
C       1.27394      2.68050      0.73541
C       0.56317      3.23948      1.72155
B      -1.02431     -0.73905     -0.10753
C      -2.05157      0.15690     -1.03228
C      -1.79662     -1.19047      1.27772
C      -2.14163     -0.04180      2.18026
C      -1.82190      0.39148     -2.49842
C      -3.37362      0.37397      2.51064
C      -1.86810      1.57102     -3.13566
H       2.94480      0.90661     -1.96477
H       0.55781      0.47159     -1.84996
H       0.73809     -1.38750      1.79495
H       3.22566     -1.45179      1.52532
H       2.69373      0.16257      1.94067
H       4.37336     -0.11843     -0.23688
H      -0.39204      2.28183     -0.54410
```

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H      1.07798     2.75299    -1.38808
H      2.03629    -2.40705    -0.82919
H      1.97757    -3.41223     0.70280
H     -0.41983    -3.74457     0.45665
H     -1.72329    -2.66826    -1.30659
H     -0.22276    -1.92042    -2.00529
H      2.35656     2.61183     0.84071
H      1.04070     3.62346     2.61911
H     -0.51917     3.33404     1.66236
H     -2.24762     1.11905    -0.53938
H     -3.00034    -0.39848    -0.95234
H     -2.71760    -1.72296     1.00178
H     -1.19848    -1.91037     1.85336
H     -1.29296     0.51253     2.58743
H     -1.63380    -0.49730    -3.10388
H     -3.53237     1.23322     3.15765
H     -4.26368    -0.13153     2.13913
H     -1.70934     1.64494    -4.20861
H     -2.06132     2.50112    -2.60397
45
bora-aza-Cope_TS-trans-2-conf11 E=-743.022596926 G=-742.708796 Imag-freq=1
C     -2.35472    -1.03932     0.59142
C     -1.30544    -0.00060     0.28038
N     -0.00874    -0.55600    -0.19551
C      0.06836    -1.88031    -0.48252
C     -1.17835    -2.68788    -0.78868
C     -2.33236    -2.26845     0.07333
C     -1.85090     0.99931    -0.78531
C      0.75000    -2.76866     1.23750
C      1.86563    -1.96013     1.45898
C      1.76634    -0.57633     1.74299
C     -3.06212     1.76972    -0.33289
C     -4.23308     1.81219    -0.97757
B      1.30262     0.18210     0.10527
C      1.29301     1.81203     0.38490
C      2.50805    -0.14807    -0.97330
C      2.23052     0.36113    -2.35755
C      0.51573     2.44910     1.49949
C      2.90667     1.31882    -3.00975
C      1.00662     2.82123     2.69200
H     -3.17484    -0.71216     1.22468
H     -1.10260     0.55980     1.19855
H      0.92166    -2.15894    -1.08786
H     -0.95786    -3.75316    -0.67340
H     -1.42128    -2.54843    -1.85440
H     -3.12674    -2.98186     0.27627
H     -2.07732     0.44301    -1.70186
H     -1.04608     1.70398    -1.02430
H     -0.16385    -2.57245     1.79240
H      0.90585    -3.80950     0.96356
H      2.83223    -2.33917     1.12675
H      2.69805    -0.06852     1.99482
H      0.93960    -0.26622     2.38340
H     -2.95080     2.34398     0.58851
H     -5.06393     2.40648    -0.60744
H     -4.39697     1.25675    -1.89877
H      1.02006     2.30113    -0.56188
H      2.35331     2.05320     0.54032
H      3.43898     0.30099    -0.60066
H      2.70393    -1.22750    -1.03609
H      1.37568    -0.09101    -2.86629
H     -0.54146     2.64616     1.31818
H      2.61942     1.64251    -4.00713
H      3.76812     1.81238    -2.56267
H      0.37569     3.27799     3.45009
H      2.05547     2.67915     2.94691
45
bora-aza-Cope_TS-trans-2-conf12 E=-743.025921288 G=-742.712697 Imag-freq=1
C      2.53960    -0.43427    -0.98743
C      1.36846     0.36802    -0.47466
N      0.25218    -0.45495     0.06753
C      0.45818    -1.77966     0.27548
C      1.86373    -2.33655     0.40206
C      2.80636    -1.66861    -0.55638
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C      1.85716     1.36470     0.62222
C     -0.21780    -2.71502    -1.42307
C     -1.47410    -2.11334    -1.50825
C     -1.64511    -0.72544    -1.72484
C      2.76679     2.43873     0.09070
C      4.00221     2.69503     0.53440
B     -1.19904     0.02874    -0.06990
C     -1.39227     1.64953    -0.29302
C     -2.22357    -0.58186     1.06503
C     -1.99450    -0.02200     2.43836
C     -2.80229     2.09743    -0.54703
C     -1.63493    -0.71494     3.52989
C     -3.25970     2.67584    -1.66722
H      3.19885     0.07249    -1.68689
H      0.96912     0.95862    -1.30594
H     -0.25795    -2.24504     0.94111
H      1.83996    -3.41989     0.25221
H      2.19908    -2.18694     1.44091
H      3.68399    -2.21037    -0.89914
H      2.35698     0.79878     1.41635
H      0.97282     1.83567     1.06488
H      0.59040    -2.33803    -2.04441
H     -0.16092    -3.77583    -1.19014
H     -2.32480    -2.67012    -1.11512
H     -2.66595    -0.37625    -1.87699
H     -0.93373    -0.24726    -2.40098
H      2.35695     3.05457    -0.71191
H      4.59947     3.50170     0.11828
H      4.45448     2.10861     1.33165
H     -0.76091     2.02981    -1.10591
H     -1.04949     2.15286     0.62442
H     -3.24269    -0.32214     0.74140
H     -2.20567    -1.67678     1.12061
H     -2.11274     1.05844     2.54401
H     -3.51515     1.93263     0.26284
H     -1.46206    -0.22561     4.48512
H     -1.50258    -1.79538     3.50164
H     -4.30191     2.96551    -1.77448
H     -2.60497     2.87530    -2.51403
45
bora-aza-Cope_TS-trans-2-conf13 E=-743.021885793 G=-742.706846 Imag-freq=1
C      2.46148    -0.61766    -1.23344
C      1.07041    -0.03982    -1.14268
N      0.41637    -0.20127     0.18344
C      1.14590    -0.69604     1.21605
C      2.66154    -0.63164     1.20869
C      3.21967    -0.86495    -0.16432
C      1.09004     1.45811    -1.58253
C      0.81038    -2.72115     1.20270
C     -0.58461    -2.70214     1.17417
C     -1.32068    -2.17411     0.08636
C      1.94360     2.36544    -0.73904
C      1.51025     3.48169    -0.14254
B     -1.11177    -0.32996     0.26551
C     -2.06108     0.31459    -0.92573
C     -1.74158     0.10986     1.72572
C     -1.64975     1.58108     2.00742
C     -1.98302    -0.12196    -2.35980
C     -2.67574     2.43341     2.15135
C     -2.82139    -0.97389    -2.97055
H      2.83863    -0.77816    -2.24105
H      0.44848    -0.56603    -1.87378
H      0.71212    -0.52649     2.19354
H      3.05814    -1.35180     1.93041
H      2.96284     0.36008     1.58188
H      4.23383    -1.24257    -0.26520
H      0.06710     1.84132    -1.61170
H      1.46538     1.47002    -2.61618
H      1.35558    -2.88265     0.27622
H      1.30941    -3.08501     2.09779
H     -1.10718    -2.83346     2.12182
H     -2.40281    -2.30246     0.12746
H     -0.91963    -2.35840    -0.91111
H      2.99204     2.08626    -0.63705
```

H 2.17919 4.11216 0.43714
H 0.47350 3.80334 -0.21662
H -1.94057 1.40700 -0.87969
H -3.08457 0.12150 -0.57671
H -2.79555 -0.19961 1.75475
H -1.25254 -0.42875 2.54926
H -0.63832 1.98713 2.08156
H -1.18299 0.30353 -2.96736
H -2.51666 3.49346 2.33331
H -3.70914 2.09635 2.08694
H -2.69749 -1.24330 -4.01628
H -3.65700 -1.42968 -2.44198
45
bora-aza-Cope_TS-trans-2-conf14 E=-743.020978914 G=-742.704737 Imag-freq=1
C 1.94123 1.78113 -1.13262
C 0.58373 1.12291 -1.09271
N 0.48551 -0.03167 -0.15847
C 1.52739 -0.29032 0.66975
C 2.52626 0.79244 1.03169
C 2.83140 1.67311 -0.14499
C -0.51192 2.19071 -0.78689
C 2.73207 -1.61252 -0.36368
C 1.76214 -2.56192 -0.67921
C 0.65773 -2.28528 -1.51775
C -0.36065 2.91615 0.52297
C -1.30447 2.98421 1.46881
B -0.47776 -1.18469 -0.45739
C -1.72944 -0.92107 -1.49890
C -0.91593 -2.07360 0.86150
C -1.46434 -1.27763 2.01212
C -3.06170 -0.51310 -0.93157
C -0.99131 -1.27933 3.26779
C -3.82441 0.51585 -1.32982
H 2.13468 2.40800 -2.00025
H 0.36584 0.74633 -2.09861
H 1.29122 -0.96364 1.48421
H 3.43330 0.33141 1.43344
H 2.10224 1.38679 1.85652
H 3.78216 2.19864 -0.17980
H -1.49447 1.71786 -0.83395
H -0.46499 2.92088 -1.60835
H 3.01975 -0.87815 -1.11103
H 3.51329 -1.87775 0.34471
H 1.69909 -3.44199 -0.03933
H 0.01482 -3.13190 -1.75783
H 0.84275 -1.63947 -2.37821
H 0.58402 3.43498 0.68449
H -1.14829 3.54345 2.38753
H -2.26397 2.48455 1.35443
H -1.89295 -1.90552 -1.96511
H -1.46973 -0.24980 -2.32758
H -1.69508 -2.77006 0.51199
H -0.10586 -2.70917 1.23862
H -2.31148 -0.62617 1.79357
H -3.45477 -1.15001 -0.13790
H -1.43062 -0.65776 4.04399
H -0.14832 -1.90418 3.55949
H -4.78826 0.72025 -0.87045
H -3.51086 1.18727 -2.12729
45
bora-aza-Cope_TS-trans-2-conf15 E=-743.024768616 G=-742.710754 Imag-freq=1
C 2.77781 -0.30108 -0.60942
C 1.43794 0.37970 -0.47509
N 0.38329 -0.45558 0.16274
C 0.73795 -1.63978 0.72185
C 2.17118 -1.90518 1.14202
C 3.14711 -1.32683 0.15974
C 1.60251 1.70553 0.33064
C 0.45729 -3.04091 -0.74826
C -0.85852 -2.71889 -1.08075
C -1.22918 -1.47586 -1.64822
C 2.41950 2.74484 -0.38764
C 3.52153 3.33010 0.09381
B -1.09369 -0.26319 -0.22006

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C     -1.48625     1.20777    -0.84812
C     -2.15243    -0.72490     0.95169
C     -1.99177     0.03813     2.23501
C     -2.79090     1.27406    -1.58875
C     -2.87841     0.88128     2.78517
C     -3.90274     1.91055    -1.19236
H      3.46155     0.13227    -1.33425
H      1.08886     0.64161    -1.48040
H      0.00281    -2.05083     1.40297
H      2.31968    -2.98146     1.26920
H      2.32078    -1.46416     2.14070
H      4.13768    -1.76649     0.07817
H      2.05031     1.47265     1.30329
H      0.60172     2.10821     0.51998
H      1.26724    -2.66781    -1.36958
H      0.65438    -3.99260    -0.26033
H     -1.64843    -3.32193    -0.63282
H     -2.27129    -1.38865    -1.95357
H     -0.53961    -1.04891    -2.37941
H      2.05482     3.03893    -1.37354
H      4.05385     4.09078    -0.47063
H      3.92442     3.06999     1.07057
H     -0.70671     1.56061    -1.53716
H     -1.52369     1.92985    -0.02019
H     -3.17207    -0.58366     0.56999
H     -2.05973    -1.79729     1.17381
H     -1.04185    -0.10357     2.75595
H     -2.82405     0.75455    -2.54817
H     -2.66533     1.40796     3.71220
H     -3.84437     1.07448     2.32205
H     -4.80775     1.90406    -1.79465
H     -3.94349     2.45512    -0.25085
45
bora-aza-Cope_TS-trans-2-conf16 E=-743.021616282 G=-742.707219 Imag-freq=1
C     -2.40212    -1.25655     0.29314
C     -1.35354    -0.17542     0.39307
N     -0.00357    -0.58441    -0.08765
C      0.11465    -1.74846    -0.77056
C     -1.08823    -2.38659    -1.43813
C     -2.31714    -2.25741    -0.58518
C     -1.81893     1.08125    -0.40208
C      0.59599    -3.17397     0.65744
C      1.67293    -2.51123     1.24264
C      1.53942    -1.28278     1.93125
C     -3.04127     1.73759     0.17869
C     -4.17546     1.98812    -0.48486
B      1.25756     0.00321     0.55820
C      1.12512     1.38289     1.44690
C      2.58640    -0.02272    -0.41439
C      2.43911     0.66607    -1.74376
C      1.22179     2.70963     0.74493
C      3.22005     1.63978    -2.23356
C      0.37755     3.74383     0.87610
H     -3.27290    -1.14067     0.93267
H     -1.25319     0.11349     1.44453
H      1.03655    -1.85440    -1.32874
H     -0.86493    -3.43293    -1.66554
H     -1.23977    -1.89538    -2.41292
H     -3.10858    -2.99585    -0.68207
H     -1.99989     0.79279    -1.44390
H     -0.99354     1.80068    -0.39410
H     -0.37995    -3.12554     1.13236
H      0.78509    -4.07784     0.08325
H      2.67286    -2.80041     0.91892
H      2.43644    -0.91051     2.42593
H      0.64094    -1.15580     2.53771
H     -2.96660     2.04191     1.22432
H     -5.01372     2.48915    -0.00844
H     -4.30016     1.70384    -1.52781
H      1.99263     1.33318     2.12422
H      0.24624     1.38732     2.10579
H      3.43278     0.42074     0.12930
H      2.88568    -1.06106    -0.61749
H      1.61163     0.32313    -2.36884
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H      2.07858     2.83475     0.08412
H      3.03795     2.07964    -3.21097
H      4.06240     2.03483    -1.66771
H      0.53334     4.67726     0.34075
H     -0.50060     3.68846     1.51747
45
bora-aza-Cope_TS-trans-2-conf17 E=-743.024541804 G=-742.709867 Imag-freq=1
C      2.38509    -0.85785    -1.49858
C      1.09228    -0.09462    -1.34129
N      0.43804    -0.25623    -0.01338
C      1.10654    -0.91506     0.96713
C      2.61708    -1.04787     0.93306
C      3.11894    -1.26972    -0.46360
C      1.33107     1.40902    -1.69042
C      0.51798    -2.88009     0.81210
C     -0.86370    -2.68794     0.77995
C     -1.51610    -1.98975    -0.26332
C      2.30004     2.13397    -0.79680
C      2.03671     3.27924    -0.15765
B     -1.09474    -0.19881     0.09505
C     -1.86221     0.64969    -1.08901
C     -1.66447     0.15828     1.59770
C     -1.45774     1.58600     2.01211
C     -3.36111     0.57430    -1.06669
C     -0.77055     2.00954     3.08389
C     -4.14184     0.05292    -2.02444
H      2.72064    -1.00742    -2.52240
H      0.39244    -0.47004    -2.09652
H      0.70448    -0.76209     1.96083
H      2.92533    -1.85610     1.60287
H      3.05149    -0.12814     1.35611
H      4.06951    -1.77596    -0.61005
H      0.37551     1.93768    -1.70463
H      1.71469     1.42207    -2.72120
H      1.04966    -3.04123    -0.12208
H      0.95788    -3.36619     1.67982
H     -1.41147    -2.82600     1.71215
H     -2.60536    -1.98618    -0.24266
H     -1.11687    -2.13182    -1.26959
H      3.29013     1.69008    -0.69546
H      2.78547     3.77196     0.45678
H      1.06483     3.76320    -0.22953
H     -1.51933     0.36024    -2.09039
H     -1.58551     1.70762    -0.96043
H     -2.74581    -0.04606     1.57219
H     -1.26546    -0.49691     2.38123
H     -1.89976     2.34576     1.36427
H     -3.85293     0.98632    -0.18376
H     -0.64913     3.06740     3.30276
H     -0.30558     1.30936     3.77616
H     -5.22440     0.03117    -1.92842
H     -3.72097    -0.37134    -2.93462
45
bora-aza-Cope_TS-trans-2-conf18 E=-743.021898814 G=-742.705843 Imag-freq=1
C      2.85450    -0.46623    -1.05467
C      1.56798     0.31748    -0.95020
N      0.57403    -0.24624     0.00782
C      0.95850    -1.28082     0.79804
C      2.42133    -1.54230     1.10040
C      3.28432    -1.29371    -0.10118
C      1.90295     1.80880    -0.63237
C      0.45031    -2.98923    -0.24355
C     -0.86572    -2.66001    -0.56464
C     -1.20507    -1.56767    -1.39783
C      2.56113     2.05040     0.69878
C      2.12956     2.91811     1.62106
B     -0.93493    -0.09003    -0.27485
C     -1.40186     1.18208    -1.21060
C     -1.87976    -0.25080     1.06308
C     -3.34903    -0.37337     0.78492
C     -1.69107     2.46462    -0.47650
C     -4.13828    -1.39909     1.13860
C     -2.84277     3.15045    -0.50789
H      3.45240    -0.26840    -1.94156
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H      1.10110     0.31821    -1.94147
H      0.30205    -1.47437     1.63628
H      2.53600    -2.56485     1.47204
H      2.72191    -0.88735     1.93361
H      4.23973    -1.80523    -0.18314
H      0.99894     2.41438    -0.71579
H      2.57886     2.14373    -1.43270
H      1.22722    -2.84740    -0.99007
H      0.63085    -3.79836     0.46027
H     -1.65640    -3.07008     0.06351
H     -2.25891    -1.47555    -1.65822
H     -0.54151    -1.36627    -2.24104
H      3.46993     1.48267     0.89710
H      2.66417     3.06453     2.55573
H      1.23267     3.51575     1.47217
H     -2.31249     0.89343    -1.75186
H     -0.65729     1.38435    -1.99361
H     -1.58881    -1.08718     1.70905
H     -1.71715     0.66621     1.65406
H     -3.80355     0.45162     0.23526
H     -0.89144     2.86234     0.15026
H     -5.19495    -1.41977     0.88355
H     -3.75212    -2.25217     1.69453
H     -2.97647     4.06656     0.06198
H     -3.69066     2.81492    -1.10298
45
bora-aza-Cope_TS-trans-2-conf19 E=-743.016205919 G=-742.700472 Imag-freq=1
C     -2.80810    -0.51301     0.95946
C     -1.48346     0.21173     0.96472
N     -0.49572    -0.29820    -0.03268
C     -0.91970    -1.20249    -0.94892
C     -2.38695    -1.33552    -1.30652
C     -3.26122    -1.19236    -0.09508
C     -1.73118     1.74460     0.81498
C     -0.55983    -3.06847    -0.08973
C      0.74878    -2.86869     0.34524
C      1.09828    -1.89391     1.30790
C     -2.44091     2.16779    -0.44342
C     -2.03628     3.14622    -1.26174
B      1.00455    -0.26491     0.31245
C      1.52688     0.82520     1.41309
C      2.00144    -0.41540    -0.98946
C      3.44666    -0.66775    -0.66603
C      1.85996     2.25336     1.03807
C      4.49333     0.09560    -1.01221
C      1.61803     2.90549    -0.10625
H     -3.41143    -0.39521     1.85686
H     -1.03562     0.07831     1.95505
H     -0.24865    -1.34790    -1.78564
H     -2.55038    -2.29397    -1.80814
H     -2.63160    -0.56281    -2.05265
H     -4.24198    -1.66063    -0.09006
H     -0.78216     2.27572     0.90673
H     -2.34602     2.03292     1.68068
H     -1.37446    -2.95266     0.61941
H     -0.74422    -3.77868    -0.89236
H      1.55088    -3.27752    -0.26955
H      2.12886    -1.90644     1.65994
H      0.38394    -1.71896     2.11399
H     -3.37097     1.64738    -0.67078
H     -2.61413     3.42425    -2.13926
H     -1.12050     3.70319    -1.07954
H      2.45837     0.40943     1.82862
H      0.86650     0.87301     2.29433
H      1.67522    -1.24541    -1.63105
H      1.93119     0.48930    -1.60784
H      3.65689    -1.57762    -0.09929
H      2.36615     2.81675     1.82705
H      5.50965    -0.17199    -0.73373
H      4.36575     1.01519    -1.58025
H      1.91461     3.94412    -0.23255
H      1.11698     2.43779    -0.94802
45
bora-aza-Cope_TS-trans-2-conf1 E=-743.024541816 G=-742.709874 Imag-freq=1
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```
C      2.38546    -0.85770    -1.49839
C      1.09250    -0.09466    -1.34134
N      0.43810    -0.25634    -0.01351
C      1.10640    -0.91518     0.96703
C      2.61692    -1.04813     0.93329
C      3.11910    -1.26966    -0.46331
C      1.33117     1.40900    -1.69044
C      0.51761    -2.88050     0.81154
C     -0.86400    -2.68809     0.77941
C     -1.51632    -1.98949    -0.26374
C      2.29975     2.13410    -0.79652
C      2.03622     3.27959    -0.15786
B     -1.09473    -0.19872     0.09487
C     -1.86206     0.64992    -1.08919
C     -1.66447     0.15837     1.59751
C     -1.45702     1.58591     2.01220
C     -3.36098     0.57504    -1.06660
C     -0.77023     2.00884     3.08446
C     -4.14203     0.05284    -2.02363
H      2.72129    -1.00704    -2.52215
H      0.39285    -0.47026    -2.09666
H      0.70406    -0.76247     1.96064
H      2.92494    -1.85656     1.60296
H      3.05129    -0.12855     1.35671
H      4.06978    -1.77575    -0.60963
H      0.37555     1.93754    -1.70500
H      1.71511     1.42206    -2.72110
H      1.04937    -3.04131    -0.12264
H      0.95746    -3.36680     1.67916
H     -1.41182    -2.82631     1.71155
H     -2.60559    -1.98588    -0.24310
H     -1.11708    -2.13153    -1.27002
H      3.28974     1.69012    -0.69451
H      2.78473     3.77240     0.45682
H      1.06443     3.76363    -0.23035
H     -1.51940     0.36012    -2.09055
H     -1.58499     1.70778    -0.96090
H     -2.74591    -0.04542     1.57175
H     -1.26595    -0.49716     2.38100
H     -1.89814     2.34605     1.36418
H     -3.85251     0.98823    -0.18405
H     -0.64827     3.06660     3.30358
H     -0.30610     1.30826     3.77690
H     -5.22458     0.03154    -1.92741
H     -3.72145    -0.37256    -2.93342
45
bora-aza-Cope_TS-trans-2-conf20 E=-743.024541812 G=-742.709872 Imag-freq=1
C     -2.38516     0.85784    -1.49854
C     -1.09237     0.09454    -1.34130
N     -0.43800     0.25626    -0.01347
C     -1.10626     0.91537     0.96695
C     -2.61678     1.04838     0.93310
C     -3.11883     1.26995    -0.46354
C     -1.33133    -1.40910    -1.69030
C     -0.51740     2.88042     0.81120
C      0.86422     2.68798     0.77917
C      1.51653     1.98930    -0.26387
C     -2.30020    -2.13392    -0.79648
C     -2.03697    -3.27931    -0.15752
B      1.09478     0.19864     0.09492
C      1.86210    -0.65019    -1.08899
C      1.66457    -0.15820     1.59762
C      1.45706    -1.58564     2.01258
C      3.36102    -0.57536    -1.06646
C      0.76963    -2.00839     3.08452
C      4.14207    -0.05364    -2.02377
H     -2.72084     1.00722    -2.52234
H     -0.39258     0.46987    -2.09663
H     -0.70403     0.76266     1.96061
H     -2.92482     1.85680     1.60277
H     -3.05124     0.12880     1.35645
H     -4.06940     1.77622    -0.60996
H     -0.37582    -1.93785    -1.70469
H     -1.71514    -1.42215    -2.72101
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H     -1.04903     3.04126    -0.12305
H     -0.95726     3.36690     1.67873
H      1.41198     2.82620     1.71134
H      2.60579     1.98541    -0.24310
H      1.11746     2.13119    -1.27024
H     -3.29018    -1.68983    -0.69485
H     -2.78570    -3.77192     0.45706
H     -1.06523    -3.76349    -0.22967
H      1.51945    -0.36059    -2.09041
H      1.58500    -1.70802    -0.96046
H      2.74603     0.04549     1.57174
H      1.26617     0.49755     2.38100
H      1.89869    -2.34590     1.36505
H      3.85259    -0.98816    -0.18375
H      0.64766    -3.06611     3.30380
H      0.30499    -1.30771     3.77649
H      5.22462    -0.03234    -1.92760
H      3.72147     0.37136    -2.93373
45
bora-aza-Cope_TS-trans-2-conf21 E=-743.024108464 G=-742.709727 Imag-freq=1
C      2.64577    -0.24800    -1.39526
C      1.21471     0.22271    -1.30008
N      0.49478    -0.23447    -0.07996
C      1.19299    -0.88653     0.88459
C      2.69630    -0.72499     1.00792
C      3.35408    -0.64950    -0.33864
C      1.16945     1.77675    -1.45150
C      1.03149    -2.87869     0.42487
C     -0.35455    -2.95222     0.28402
C     -1.06433    -2.25359    -0.72127
C      1.88318     2.55193    -0.37779
C      1.33276     3.53260     0.34670
B     -1.02284    -0.46780    -0.12199
C     -1.84530     0.38740    -1.26399
C     -1.76775    -0.42023     1.34349
C     -1.75812     0.93337     1.99062
C     -3.27657    -0.01566    -1.47369
C     -1.24557     1.23517     3.19364
C     -4.35897     0.72461    -1.19310
H      3.09464    -0.18696    -2.38419
H      0.67611    -0.17902    -2.16648
H      0.68097    -0.94844     1.83684
H      3.10220    -1.54578     1.60659
H      2.89557     0.19167     1.58539
H      4.39786    -0.93715    -0.43406
H      0.13107     2.10813    -1.51694
H      1.63400     1.99883    -2.42344
H      1.64932    -2.80035    -0.46588
H      1.49815    -3.39231     1.26219
H     -0.92516    -3.32428     1.13479
H     -2.12900    -2.47365    -0.78975
H     -0.58484    -2.18318    -1.69959
H      2.92961     2.29745    -0.21080
H      1.90449     4.07661     1.09378
H      0.29310     3.82537     0.21521
H     -1.33759     0.31282    -2.23650
H     -1.82954     1.45086    -0.98777
H     -2.81306    -0.70670     1.15237
H     -1.38202    -1.15736     2.05807
H     -2.19956     1.74630     1.41094
H     -3.44125    -1.00631    -1.90136
H     -1.26029     2.25027     3.58252
H     -0.79365     0.47429     3.82830
H     -5.36496     0.35386    -1.37258
H     -4.27273     1.72460    -0.77118
45
bora-aza-Cope_TS-trans-2-conf22 E=-743.019659639 G=-742.704737 Imag-freq=1
C      2.91653    -0.05639    -1.02514
C      1.50702     0.48069    -0.95086
N      0.62643    -0.21915     0.02958
C      1.19364    -1.12740     0.86311
C      2.67696    -1.09608     1.17630
C      3.48731    -0.74569    -0.03648
C      1.56222     2.01958    -0.69497
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C      1.02838    -2.94697    -0.10645
C     -0.31833    -2.88543    -0.46119
C     -0.83665    -1.90680    -1.34208
C      2.14817     2.43068     0.62835
C      1.55266     3.23786     1.51355
B     -0.88366    -0.35781    -0.26447
C     -1.56702     0.75911    -1.25496
C     -1.79906    -0.65147     1.07060
C     -3.17476    -1.20090     0.81721
C     -2.04604     2.02909    -0.59844
C     -4.34097    -0.65399     1.18843
C     -3.26164     2.57710    -0.73333
H      3.47165     0.20864    -1.92218
H      1.05384     0.35691    -1.94040
H      0.57960    -1.40947     1.70825
H      2.97758    -2.06119     1.59477
H      2.84286    -0.35918     1.97816
H      4.52130    -1.07469    -0.09752
H      0.56553     2.44768    -0.81114
H      2.17793     2.43748    -1.50473
H      1.78077    -2.69139    -0.84749
H      1.34179    -3.67857     0.63451
H     -1.02833    -3.42179     0.16891
H     -1.87667    -2.02739    -1.64256
H     -0.19575    -1.60556    -2.17261
H      3.14415     2.04980     0.85306
H      2.04011     3.51653     2.44391
H      0.56216     3.65214     1.33776
H     -2.43176     0.29302    -1.74571
H     -0.88362     1.02589    -2.07482
H     -1.30043    -1.36377     1.74251
H     -1.89109     0.28562     1.63963
H     -3.21706    -2.15682     0.29075
H     -1.33704     2.54668     0.04911
H     -5.29063    -1.13454     0.96614
H     -4.38306     0.29482     1.71936
H     -3.53077     3.49918    -0.22384
H     -4.03023     2.11518    -1.35065
45
bora-aza-Cope_TS-trans-2-conf23 E=-743.022648757 G=-742.708603 Imag-freq=1
C     -2.00653    -1.20519     1.07706
C     -1.25418    -0.11178     0.35913
N      0.14313    -0.46555    -0.01086
C      0.55683    -1.74914     0.14499
C     -0.44344    -2.88723     0.21948
C     -1.67008    -2.49313     0.98831
C     -2.03046     0.30595    -0.92788
C      1.42657    -1.81512     1.99664
C      2.29961    -0.73457     1.85834
C      1.85035     0.59623     1.68018
C     -3.39930     0.87036    -0.65782
C     -4.53997     0.40871    -1.18165
B      1.22548     0.61665    -0.07745
C      0.80316     2.19420    -0.35386
C      2.49041     0.23120    -1.06840
C      2.12492     0.17019    -2.52264
C     -0.09888     2.96886     0.56318
C      2.22780    -0.90259    -3.32255
C      0.29564     3.84161     1.50307
H     -2.88571    -0.89185     1.63345
H     -1.20604     0.75689     1.02353
H      1.45437    -1.99757    -0.40696
H      0.03879    -3.76644     0.65684
H     -0.70910    -3.17540    -0.81027
H     -2.25819    -3.26551     1.47702
H     -2.10387    -0.56520    -1.58847
H     -1.42967     1.05893    -1.45071
H      0.48931    -1.67178     2.52821
H      1.84461    -2.81659     2.06783
H      3.33411    -0.95724     1.59689
H      2.62006     1.36892     1.67797
H      0.96539     0.89468     2.24342
H     -3.44125     1.73377     0.00848
H     -5.49589     0.87628    -0.96230
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H     -4.55366     -0.44977     -1.85009
H      0.39471      2.25545     -1.37389
H      1.76566      2.72185     -0.39176
H      3.24096      1.02399     -0.92543
H      2.99242     -0.70380     -0.79175
H      1.71871      1.08602     -2.95654
H     -1.17294      2.82380      0.44317
H      1.91479     -0.87082     -4.36318
H      2.63053     -1.84743     -2.96083
H     -0.42089      4.36444      2.13121
H      1.34864      4.05874      1.67410
45
bora-aza-Cope_TS-trans-2-conf24 E=-743.013021628 G=-742.698369 Imag-freq=1
C     -2.05792     -1.78816     -0.88613
C     -0.69183     -1.16235     -1.03558
N     -0.44795      0.00809     -0.14155
C     -1.39505      0.32686      0.77247
C     -2.37341     -0.70816      1.28989
C     -2.82342     -1.63010      0.19459
C      0.39366     -2.26997     -0.87780
C     -2.70581      1.61753     -0.23243
C     -1.76096      2.52347     -0.70383
C     -0.74241      2.17443     -1.62061
C      0.40481     -2.97989      0.45074
C      1.50270     -3.30458      1.14322
B      0.49917      1.12822     -0.58946
C      1.61979      0.81230     -1.74551
C      1.03260      2.14254      0.60840
C      1.59473      1.53382      1.86177
C      3.01626      0.30651     -1.44832
C      1.10181      1.68752      3.10097
C      3.46290     -0.38911     -0.39496
H     -2.36258     -2.44150     -1.70072
H     -0.60221     -0.80136     -2.06676
H     -1.07422      1.04783      1.51279
H     -3.22155     -0.20240      1.76072
H     -1.88087     -1.27571      2.09582
H     -3.77855     -2.13974      0.29081
H      1.37995     -1.85543     -1.09407
H      0.18158     -3.00570     -1.66797
H     -3.06682      0.83100     -0.88866
H     -3.40828      1.93966      0.53244
H     -1.63388      3.44715     -0.13960
H     -0.12055      2.99405     -1.97965
H     -1.01144      1.47208     -2.41158
H     -0.56622     -3.28007      0.84351
H      1.43725     -3.85199      2.07976
H      2.49990     -3.04415      0.79713
H      1.76769      1.77092     -2.26434
H      1.21227      0.16517     -2.54016
H      1.82502      2.74596      0.13837
H      0.25703      2.85685      0.90765
H      2.48348      0.91620      1.74689
H      3.74721      0.53012     -2.22990
H      1.56231      1.20766      3.96101
H      0.22382      2.30181      3.29665
H      4.50097     -0.70695     -0.33226
H      2.81781     -0.67509      0.42884
45
bora-aza-Cope_TS-trans-2-conf25 E=-743.024768607 G=-742.710752 Imag-freq=1
C     -2.77775      0.30125     -0.60961
C     -1.43793     -0.37961     -0.47518
N     -0.38329      0.45558      0.16275
C     -0.73793      1.63977      0.72192
C     -2.17118      1.90520      1.14200
C     -3.14706      1.32697      0.15961
C     -1.60264     -1.70545      0.33053
C     -0.45705      3.04097     -0.74797
C      0.85879      2.71895     -1.08032
C      1.22946      1.47596     -1.64788
C     -2.41972     -2.74467     -0.38779
C     -3.52178     -3.32988      0.09367
B      1.09372      0.26313     -0.21999
C      1.48620     -1.20783     -0.84814
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C      2.15241     0.72459     0.95189
C      1.99170    -0.03871     2.23504
C      2.79070    -1.27404    -1.58904
C      2.87829    -0.88201     2.78505
C      3.90286    -1.90994    -1.19260
H     -3.46145    -0.13199    -1.33453
H     -1.08879    -0.64153    -1.48046
H     -0.00283     2.05069     1.40317
H     -2.31965     2.98148     1.26924
H     -2.32088     1.46412     2.14065
H     -4.13760     1.76669     0.07798
H     -2.05043    -1.47254     1.30318
H     -0.60189    -2.10822     0.51987
H     -1.26693     2.66797    -1.36945
H     -0.65418     3.99263    -0.25999
H      1.64866     3.32190    -0.63218
H      2.27161     1.38868    -1.95307
H      0.53999     1.04917    -2.37927
H     -2.05508    -3.03873    -1.37370
H     -4.05415    -4.09051    -0.47079
H     -3.92463    -3.06980     1.07045
H      0.70654    -1.56071    -1.53702
H      1.52384    -1.92988    -0.02020
H      3.17206     0.58343     0.57019
H      2.05972     1.79693     1.17424
H      1.04177     0.10293     2.75600
H      2.82344    -0.75499    -2.54872
H      2.66517    -1.40886     3.71198
H      3.84424    -1.07516     2.32191
H      4.80773    -1.90342    -1.79509
H      3.94401    -2.45405    -0.25084
45
bora-aza-Cope_TS-trans-2-conf26 E=-743.024108457 G=-742.709726 Imag-freq=1
C      2.64572    -0.24781    -1.39533
C      1.21464     0.22283    -1.30009
N      0.49477    -0.23442    -0.07997
C      1.19303    -0.88649     0.88455
C      2.69634    -0.72484     1.00784
C      3.35407    -0.64931    -0.33874
C      1.16933     1.77688    -1.45145
C      1.03166    -2.87864     0.42482
C     -0.35437    -2.95225     0.28385
C     -1.06409    -2.25362    -0.72146
C      1.88304     2.55201    -0.37770
C      1.33254     3.53250     0.34697
B     -1.02284    -0.46779    -0.12204
C     -1.84534     0.38741    -1.26400
C     -1.76775    -0.42043     1.34344
C     -1.75808     0.93310     1.99074
C     -3.27663    -0.01564    -1.47362
C     -1.24555     1.23473     3.19380
C     -4.35901     0.72467    -1.19306
H      3.09455    -0.18675    -2.38428
H      0.67603    -0.17891    -2.16648
H      0.68104    -0.94843     1.83682
H      3.10231    -1.54561     1.60649
H      2.89556     0.19183     1.58530
H      4.39786    -0.93693    -0.43420
H      0.13094     2.10823    -1.51688
H      1.63387     1.99901    -2.42339
H      1.64957    -2.80025    -0.46586
H      1.49827    -3.39226     1.26218
H     -0.92504    -3.32439     1.13455
H     -2.12875    -2.47369    -0.79007
H     -0.58446    -2.18299    -1.69970
H      2.92951     2.29764    -0.21081
H      1.90423     4.07648     1.09410
H      0.29282     3.82513     0.21560
H     -1.33768     0.31277    -2.23654
H     -1.82954     1.45088    -0.98785
H     -2.81306    -0.70686     1.15229
H     -1.38201    -1.15765     2.05792
H     -2.19947     1.74612     1.41114
H     -3.44134    -1.00632    -1.90121
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H     -1.26023     2.24979     3.58280
H     -0.79368     0.47376     3.82838
H     -5.36500     0.35391    -1.37248
H     -4.27275     1.72469    -0.77123
45
bora-aza-Cope_TS-trans-2-conf27 E=-743.021885811 G=-742.706845 Imag-freq=1
C      2.46138    -0.61804    -1.23332
C      1.07039    -0.04001    -1.14264
N      0.41630    -0.20129     0.18348
C      1.14578    -0.69598     1.21617
C      2.66142    -0.63170     1.20881
C      3.21954    -0.86528    -0.16416
C      1.09021     1.45789    -1.58259
C      0.81007    -2.72104     1.20311
C     -0.58493    -2.70192     1.17461
C     -1.32096    -2.17400     0.08672
C      1.94402     2.36515    -0.73927
C      1.51087     3.48142    -0.14266
B     -1.11182    -0.32983     0.26551
C     -2.06103     0.31460    -0.92589
C     -1.74166     0.11035     1.72560
C     -1.64981     1.58163     2.00696
C     -1.98289    -0.12213    -2.35990
C     -2.67580     2.43399     2.15080
C     -2.82112    -0.97427    -2.97056
H      2.83852    -0.77873    -2.24091
H      0.44840    -0.56618    -1.87372
H      0.71200    -0.52625     2.19363
H      3.05796    -1.35177     1.93065
H      2.96281     0.36006     1.58183
H      4.23365    -1.24305    -0.26497
H      0.06733     1.84125    -1.61165
H      1.46543     1.46968    -2.61628
H      1.35522    -2.88273     0.27664
H      1.30909    -3.08483     2.09825
H     -1.10750    -2.83305     2.12229
H     -2.40310    -2.30222     0.12786
H     -0.91995    -2.35853    -0.91073
H      2.99246     2.08590    -0.63750
H      2.17998     4.11184     0.43689
H      0.47413     3.80316    -0.21652
H     -1.94050     1.40700    -0.87996
H     -3.08455     0.12157    -0.57691
H     -2.79563    -0.19911     1.75470
H     -1.25263    -0.42807     2.54928
H     -0.63838     1.98771     2.08090
H     -1.18291     0.30340    -2.96750
H     -2.51671     3.49408     2.33251
H     -3.70921     2.09690     2.08657
H     -2.69716    -1.24379    -4.01625
H     -3.65667    -1.43011    -2.44194
45
bora-aza-Cope_TS-trans-2-conf28 E=-743.020559381 G=-742.706401 Imag-freq=1
C      2.80207    -0.14364    -0.32804
C      1.40455     0.41715    -0.42501
N      0.33809    -0.48710     0.09026
C      0.70664    -1.62119     0.73254
C      2.07528    -1.75440     1.37007
C      3.13694    -1.11080     0.52750
C      1.33816     1.77913     0.33018
C      0.79131    -3.07618    -0.74734
C     -0.48512    -2.88577    -1.27142
C     -0.88804    -1.68816    -1.90937
C      2.17482     2.85765    -0.30287
C      3.13763     3.55057     0.31472
B     -1.08077    -0.43154    -0.50125
C     -1.51986     0.91988    -1.33669
C     -2.24902    -0.99503     0.51162
C     -2.27746    -0.36632     1.87864
C     -2.27595     1.99577    -0.60517
C     -3.31959     0.23689     2.46784
C     -3.48501     2.46577    -0.94512
H      3.54892     0.33331    -0.95677
H      1.18943     0.61036    -1.48216
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H     -0.08647    -2.09883     1.29383
H      2.29148    -2.81157     1.54975
H      2.03484    -1.28556     2.36665
H      4.16296    -1.45839     0.61432
H      1.64194     1.62032     1.37100
H      0.29311     2.10323     0.34317
H      1.64477    -2.62140    -1.24269
H      1.00641    -3.99652    -0.20975
H     -1.26909    -3.56298    -0.93219
H     -1.88092    -1.69771    -2.35867
H     -0.14605    -1.19634    -2.54143
H      1.94848     3.08501    -1.34618
H      3.69129     4.33330    -0.19647
H      3.40021     3.35992     1.35332
H     -2.15554     0.59179    -2.17010
H     -0.64330     1.38081    -1.81485
H     -3.22769    -0.85718     0.03162
H     -2.14213    -2.08053     0.65219
H     -1.34667    -0.42211     2.44744
H     -1.79825     2.43020     0.27415
H     -3.24278     0.65843     3.46720
H     -4.27948     0.33905     1.96512
H     -3.97658     3.24675    -0.37027
H     -4.02580     2.07605    -1.80628
45
bora-aza-Cope_TS-trans-2-conf29 E=-743.020874764 G=-742.706854 Imag-freq=1
C     -2.77754     0.22244    -1.28838
C     -1.46070    -0.45881    -1.00607
N     -0.65451     0.17050     0.07510
C     -1.22450     1.15234     0.82166
C     -2.73236     1.30142     0.90819
C     -3.39452     1.00897    -0.40549
C     -1.70251    -1.97508    -0.71606
C     -0.67887     2.90933    -0.06919
C      0.69647     2.68551    -0.14584
C      1.26323     1.65586    -0.93355
C     -2.52865    -2.27162     0.50556
C     -2.13228    -3.04545     1.52246
B      0.88789     0.09873     0.03058
C      1.50762    -1.13435    -0.87346
C      1.54546     0.18653     1.54027
C      3.03775     0.29067     1.65830
C      2.90509    -0.95940    -1.39590
C      3.84644    -0.56486     2.30063
C      3.26021    -0.95296    -2.68963
H     -3.22995    -0.00969    -2.24996
H     -0.86767    -0.41596    -1.92587
H     -0.72364     1.35230     1.76020
H     -2.97598     2.30603     1.26627
H     -3.09938     0.61176     1.68468
H     -4.36367     1.45139    -0.62067
H     -0.73995    -2.48628    -0.63991
H     -2.21044    -2.38045    -1.60332
H     -1.28944     2.74538    -0.95352
H     -1.04518     3.68097     0.60388
H      1.31984     3.12385     0.63409
H      2.34988     1.64467    -1.00684
H      0.78393     1.45488    -1.89380
H     -3.52496    -1.83092     0.53626
H     -2.77985    -3.24258     2.37262
H     -1.14857    -3.51061     1.53634
H      0.87265    -1.38196    -1.73121
H      1.50221    -2.02181    -0.21794
H      1.13498     1.04999     2.08225
H      1.21064    -0.70505     2.09346
H      3.49666     1.16119     1.18363
H      3.68827    -0.82739    -0.65066
H      4.92195    -0.41195     2.34260
H      3.45668    -1.45148     2.79821
H      4.29436    -0.81542    -2.99583
H      2.52686    -1.08122    -3.48460
45
bora-aza-Cope_TS-trans-2-conf2 E=-743.021885803 G=-742.706847 Imag-freq=1
C      2.46157    -0.61738    -1.23356
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C      1.07045    -0.03970    -1.14275
N      0.41648    -0.20123     0.18340
C      1.14609    -0.69600     1.21595
C      2.66171    -0.63146     1.20855
C      3.21982    -0.86464    -0.16448
C      1.08991     1.45823    -1.58261
C      0.81072    -2.72114     1.20248
C     -0.58428    -2.70226     1.17398
C     -1.32042    -2.17424     0.08623
C      1.94320     2.36568    -0.73898
C      1.50961     3.48189    -0.14258
B     -1.11163    -0.33005     0.26555
C     -2.06107     0.31450    -0.92558
C     -1.74141     0.10959     1.72584
C     -1.64973     1.58079     2.00764
C     -1.98323    -0.12213    -2.35963
C     -2.67580     2.43302     2.15161
C     -2.82189    -0.97383    -2.97029
H      2.83871    -0.77781    -2.24119
H      0.44854    -0.56598    -1.87383
H      0.71231    -0.52655     2.19347
H      3.05840    -1.35162     1.93023
H      2.96294     0.36027     1.58178
H      4.23402    -1.24216    -0.26541
H      0.06692     1.84129    -1.61196
H      1.46542     1.47019    -2.61619
H      1.35590    -2.88254     0.27597
H      1.30981    -3.08502     2.09754
H     -1.10682    -2.83371     2.12163
H     -2.40254    -2.30266     0.12733
H     -0.91936    -2.35838    -0.91127
H      2.99166     2.08664    -0.63680
H      2.17836     4.11246     0.43720
H      0.47283     3.80341    -0.21686
H     -1.94048     1.40690    -0.87960
H     -3.08453     0.12149    -0.57643
H     -2.79534    -0.20001     1.75490
H     -1.25226    -0.42903     2.54932
H     -0.63834     1.98694     2.08183
H     -1.18310     0.30309    -2.96727
H     -2.51683     3.49307     2.33365
H     -3.70918     2.09586     2.08717
H     -2.69813    -1.24333    -4.01602
H     -3.65760    -1.42935    -2.44165
45
bora-aza-Cope_TS-trans-2-conf30 E=-743.014883502 G=-742.699914 Imag-freq=1
C     -2.02477    -1.76121     0.14423
C     -1.33762    -0.43928     0.38391
N      0.09872    -0.40591    -0.02406
C      0.62201    -1.50164    -0.62226
C     -0.24961    -2.47465    -1.38864
C     -1.56904    -2.68207    -0.70630
C     -2.13465     0.68432    -0.34027
C      1.27425    -2.70794     0.96211
C      2.04510    -1.75695     1.62425
C      1.50583    -0.57926     2.19421
C     -3.52396     0.87665     0.20466
C     -4.65048     0.84002    -0.51550
B      1.07762     0.53362     0.69002
C      0.48998     1.85488     1.46427
C      2.52063     0.79180    -0.08357
C      2.49062     1.21695    -1.52422
C      0.29149     3.20444     0.80241
C      3.00065     0.53033    -2.55904
C      0.07567     3.50724    -0.48476
H     -2.97083    -1.89711     0.66101
H     -1.37392    -0.22473     1.45968
H      1.60030    -1.34516    -1.05679
H      0.28667    -3.41966    -1.51765
H     -0.39622    -2.07501    -2.40516
H     -2.12466    -3.59616    -0.89867
H     -2.17229     0.45912    -1.41237
H     -1.58307     1.61955    -0.21922
H      0.26121    -2.90621     1.30020
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H      1.77224    -3.54629     0.48095
H      3.12115    -1.78455     1.45386
H      2.20208     0.03915     2.76039
H      0.53276    -0.66942     2.68032
H     -3.59024     1.08380     1.27452
H     -5.62146     1.01659    -0.06094
H     -4.63712     0.63649    -1.58437
H      1.19868     2.04049     2.28471
H     -0.44763     1.62660     1.99839
H      3.01510     1.58702     0.49626
H      3.18057    -0.08012    -0.00905
H      2.01281     2.17077    -1.73904
H      0.30045     4.04516     1.50107
H      2.93357     0.90267    -3.57829
H      3.50697    -0.42411    -2.42055
H     -0.07775     4.53732    -0.79737
H      0.03488     2.75527    -1.26647
45
bora-aza-Cope_TS-trans-2-conf31 E=-743.022047833 G=-742.706807 Imag-freq=1
C      2.15937     0.22034    -1.63169
C      0.85945     0.67625    -1.01642
N      0.24061    -0.30896    -0.08923
C      0.95513    -1.40227     0.28382
C      2.46778    -1.42256     0.16081
C      2.92978    -0.72113    -1.08356
C      1.05489     2.06065    -0.32340
C      0.41562    -2.88923    -1.01147
C     -0.97264    -2.78149    -0.90853
C     -1.67661    -1.62695    -1.32201
C      2.04719     2.09078     0.80665
C      1.78709     2.54595     2.03747
B     -1.28272    -0.37938     0.03579
C     -2.18772     0.94816    -0.33783
C     -1.81891    -1.02574     1.45638
C     -1.61387    -0.13948     2.65018
C     -2.24612     1.51450    -1.72888
C     -0.89735    -0.43762     3.74494
C     -2.08749     2.80049    -2.07546
H      2.46687     0.74618    -2.53295
H      0.14413     0.85229    -1.82580
H      0.58318    -1.89695     1.17254
H      2.82084    -2.45751     0.19232
H      2.89020    -0.93607     1.05416
H      3.88297    -1.00053    -1.52492
H      0.08589     2.42584     0.02428
H      1.38823     2.75103    -1.11199
H      0.91594    -2.43597    -1.86347
H      0.89961    -3.77989    -0.61750
H     -1.48356    -3.47487    -0.24087
H     -2.76539    -1.68285    -1.29372
H     -1.30178    -1.13350    -2.21914
H      3.05185     1.73524     0.57849
H      2.55223     2.56707     2.80896
H      0.80143     2.91477     2.31369
H     -1.96836     1.76186     0.36786
H     -3.21360     0.62777    -0.09352
H     -2.89997    -1.18898     1.32253
H     -1.39643    -2.01350     1.67637
H     -2.08269     0.84549     2.60563
H     -2.47649     0.80539    -2.52608
H     -0.77730     0.27192     4.55977
H     -0.40636    -1.40281     3.85971
H     -2.16866     3.12510    -3.10979
H     -1.86692     3.56921    -1.33690
45
bora-aza-Cope_TS-trans-2-conf32 E=-743.020978934 G=-742.704736 Imag-freq=1
C      1.94106     1.78136    -1.13253
C      0.58363     1.12300    -1.09266
N      0.48551    -0.03163    -0.15846
C      1.52744    -0.29024     0.66972
C      2.52624     0.79257     1.03170
C      2.83127     1.67335    -0.14492
C     -0.51212     2.19067    -0.78684
C      2.73220    -1.61228    -0.36380
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C      1.76233    -2.56175    -0.67934
C      0.65789    -2.28518    -1.51784
C     -0.36094     2.91609     0.52304
C     -1.30478     2.98406     1.46887
B     -0.47767    -1.18469    -0.45741
C     -1.72938    -0.92113    -1.49889
C     -0.91574    -2.07370     0.86144
C     -1.46416    -1.27784     2.01212
C     -3.06166    -0.51325    -0.93153
C     -0.99112    -1.27960     3.26778
C     -3.82447     0.51562    -1.32979
H      2.13443     2.40832    -2.00012
H      0.36583     0.74641    -2.09858
H      1.29134    -0.96362     1.48415
H      3.43333     0.33159     1.43339
H      2.10220     1.38684     1.85658
H      3.78197     2.19899    -0.17972
H     -1.49463     1.71774    -0.83393
H     -0.46524     2.92087    -1.60828
H      3.01980    -0.87787    -1.11112
H      3.51346    -1.87748     0.34456
H      1.69938    -3.44185    -0.03950
H      0.01501    -3.13184    -1.75789
H      0.84279    -1.63934    -2.37830
H      0.58369     3.43499     0.68460
H     -1.14867     3.54329     2.38760
H     -2.26426     2.48436     1.35444
H     -1.89285    -1.90559    -1.96510
H     -1.46973    -0.24984    -2.32757
H     -1.69484    -2.77020     0.51191
H     -0.10561    -2.70925     1.23850
H     -2.31133    -0.62639     1.79363
H     -3.45464    -1.15016    -0.13782
H     -1.43045    -0.65811     4.04403
H     -0.14810    -1.90444     3.55943
H     -4.78832     0.71996    -0.87040
H     -3.51100     1.18703    -2.12730
45
bora-aza-Cope_TS-trans-2-conf33 E=-743.021951020 G=-742.708212 Imag-freq=1
C     -2.70855    -0.83482     0.73436
C     -1.66041     0.17795     0.34029
N     -0.41693    -0.41400    -0.22899
C     -0.43240    -1.72112    -0.59218
C     -1.74380    -2.44482    -0.83664
C     -2.78720    -2.03792     0.16304
C     -2.26718     1.18666    -0.68500
C      0.33373    -2.75503     1.00411
C      1.50625    -2.01628     1.15207
C      1.51145    -0.65518     1.54269
C     -3.33937     2.06304    -0.09701
C     -4.59080     2.16824    -0.55710
B      0.95062     0.26164     0.01825
C      0.86124     1.84019     0.48630
C      2.00894     0.04224    -1.23122
C      3.46807    -0.06748    -0.89687
C      2.15569     2.50248     0.86007
C      4.26762    -1.10637    -1.18274
C      2.71304     3.55418     0.24242
H     -3.44094    -0.50916     1.46798
H     -1.37977     0.74158     1.23485
H      0.35624    -2.01117    -1.27486
H     -1.57062    -3.52461    -0.82115
H     -2.07734    -2.21096    -1.86054
H     -3.57792    -2.73796     0.41960
H     -2.65868     0.62659    -1.54165
H     -1.45259     1.81950    -1.05407
H     -0.50962    -2.54986     1.65824
H      0.40199    -3.78038     0.64826
H      2.40919    -2.40117     0.67849
H      2.49340    -0.22419     1.73717
H      0.76852    -0.36341     2.28744
H     -3.04337     2.66154     0.76647
H     -5.31188     2.83681    -0.09486
H     -4.93325     1.59166    -1.41403
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H      0.18865     1.94172     1.35077
H      0.41043     2.42417    -0.32863
H      1.74095    -0.81749    -1.85797
H      1.87674     0.93076    -1.87190
H      3.90386     0.78036    -0.36807
H      2.67845     2.08886     1.72477
H      5.31609    -1.11539    -0.89506
H      3.89782    -1.98269    -1.71335
H      3.65712     3.97730     0.57629
H      2.24399     4.02157    -0.62189
45
bora-aza-Cope_TS-trans-2-conf34 E=-743.023499687 G=-742.708629 Imag-freq=1
C      2.76017    -0.13174    -1.27197
C      1.30072     0.24948    -1.21895
N      0.58234    -0.22007    -0.00251
C      1.30057    -0.79151     0.99752
C      2.78717    -0.52794     1.14544
C      3.46888    -0.45534    -0.18931
C      1.15607     1.79328    -1.40794
C      1.27650    -2.80672     0.60728
C     -0.10092    -2.96899     0.46022
C     -0.84253    -2.35770    -0.57866
C      1.81221     2.63728    -0.34932
C      1.19176     3.58547     0.36176
B     -0.91985    -0.54710    -0.07281
C     -1.76245     0.20485    -1.27064
C     -1.69768    -0.45900     1.37347
C     -1.68903     0.91281     1.98489
C     -3.10932    -0.37752    -1.59031
C     -2.75487     1.69115     2.22487
C     -4.30131     0.19165    -1.35851
H      3.22523    -0.07339    -2.25355
H      0.80889    -0.20797    -2.08503
H      0.77576    -0.85916     1.94262
H      3.23121    -1.29922     1.78152
H      2.91312     0.41945     1.69331
H      4.53020    -0.68039    -0.25411
H      0.09776     2.05271    -1.48312
H      1.60988     2.02367    -2.38299
H      1.89712    -2.72088    -0.28082
H      1.76633    -3.25731     1.46731
H     -0.65551    -3.33898     1.32262
H     -1.89122    -2.64518    -0.64280
H     -0.36013    -2.30434    -1.55683
H      2.87490     2.46383    -0.18134
H      1.72327     4.18235     1.09814
H      0.13296     3.79787     0.22916
H     -1.18576     0.21201    -2.20604
H     -1.90201     1.25517    -0.97882
H     -2.73622    -0.78335     1.22623
H     -1.26537    -1.16106     2.10030
H     -0.70530     1.31190     2.24223
H     -3.10605    -1.35889    -2.06819
H     -2.65087     2.68306     2.65791
H     -3.76554     1.36176     1.99046
H     -5.23076    -0.30551    -1.62463
H     -4.38458     1.17098    -0.89102
45
bora-aza-Cope_TS-trans-2-conf35 E=-743.022853508 G=-742.707717 Imag-freq=1
C     -2.63682    -0.71180     0.43569
C     -1.42576     0.18862     0.45492
N     -0.16777    -0.46101    -0.00813
C     -0.23811    -1.70122    -0.55051
C     -1.53087    -2.21825    -1.15087
C     -2.71903    -1.79641    -0.33688
C     -1.70911     1.45251    -0.41213
C      0.02890    -2.99809     1.03592
C      1.20872    -2.45539     1.54179
C      1.29137    -1.14655     2.07362
C     -2.79053     2.33561     0.14873
C     -3.89689     2.71022    -0.50260
B      1.18917    -0.01890     0.55206
C      1.29961     1.47715     1.24155
C      2.47864    -0.38005    -0.40899
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C      2.37730     0.13820    -1.81442
C      1.74917     2.61727     0.37003
C      2.40755    -0.60060    -2.93470
C      2.90171     3.29157     0.49565
H     -3.47806    -0.38984     1.04330
H     -1.26422     0.52170     1.48677
H      0.65046    -1.99972    -1.09211
H     -1.47757    -3.30661    -1.24788
H     -1.60901    -1.83100    -2.17952
H     -3.62453    -2.39634    -0.37366
H     -1.96440     1.13312    -1.42876
H     -0.78080     2.02758    -0.47690
H     -0.91826    -2.73724     1.50003
H      0.06060    -3.98439     0.57906
H      2.14221    -2.94183     1.25926
H      2.24784    -0.87036     2.51698
H      0.43958    -0.80012     2.66204
H     -2.62871     2.69952     1.16501
H     -4.62983     3.36906    -0.04514
H     -4.10320     2.37292    -1.51633
H      2.02683     1.39010     2.05970
H      0.35187     1.75750     1.72274
H      3.34927     0.09021     0.07457
H      2.70068    -1.45325    -0.44764
H      2.25073     1.21595    -1.92122
H      1.08145     2.91702    -0.43987
H      2.30592    -0.14919    -3.91853
H      2.53882    -1.68138    -2.90380
H      3.16668     4.10006    -0.18101
H      3.61912     3.05133     1.27868
45
bora-aza-Cope_TS-trans-2-conf36 E=-743.021616303 G=-742.707220 Imag-freq=1
C     -2.40234    -1.25639     0.29273
C     -1.35363    -0.17542     0.39299
N     -0.00365    -0.58448    -0.08766
C      0.11458    -1.74856    -0.77050
C     -1.08823    -2.38663    -1.43826
C     -2.31731    -2.25725    -0.58559
C     -1.81877     1.08148    -0.40193
C      0.59558    -3.17404     0.65769
C      1.67254    -2.51136     1.24289
C      1.53913    -1.28281     1.93139
C     -3.04100     1.73794     0.17894
C     -4.17516     1.98875    -0.48456
B      1.25749     0.00311     0.55826
C      1.12503     1.38285     1.44687
C      2.58638    -0.02292    -0.41426
C      2.43914     0.66568    -1.74373
C      1.22225     2.70952     0.74485
C      3.22003     1.63939    -2.23361
C      0.37819     3.74391     0.87562
H     -3.27326    -1.14038     0.93203
H     -1.25336     0.11322     1.44454
H      1.03656    -1.85459    -1.32851
H     -0.86499    -3.43301    -1.66553
H     -1.23951    -1.89548    -2.41313
H     -3.10886    -2.99554    -0.68269
H     -1.99978     0.79323    -1.44381
H     -0.99325     1.80076    -0.39384
H     -0.38041    -3.12544     1.13250
H      0.78463    -4.07798     0.08360
H      2.67246    -2.80069     0.91929
H      2.43616    -0.91066     2.42614
H      0.64063    -1.15569     2.53779
H     -2.96627     2.04210     1.22462
H     -5.01333     2.48984    -0.00807
H     -4.29992     1.70463    -1.52754
H      1.99229     1.33299     2.12452
H      0.24591     1.38751     2.10543
H      3.43271     0.42065     0.12941
H      2.88571    -1.06128    -0.61718
H      1.61174     0.32258    -2.36884
H      2.07933     2.83443     0.08438
H      3.03796     2.07910    -3.21109
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H      4.06230     2.03458    -1.66775
H      0.53438     4.67728     0.34026
H     -0.50022     3.68878     1.51666
45
bora-aza-Cope_TS-trans-2-conf37 E=-743.019387790 G=-742.703772 Imag-freq=1
C      2.69124     0.85395    -1.04058
C      1.18876     0.72192    -1.10300
N      0.60026    -0.16411    -0.05944
C      1.41683    -0.65632     0.90372
C      2.71670     0.03333     1.26723
C      3.40528     0.58233     0.05258
C      0.54586     2.14360    -1.08389
C      2.11763    -2.46291     0.14965
C      0.88663    -3.03116    -0.16915
C      0.01853    -2.49426    -1.14927
C      0.79754     2.94777     0.16270
C     -0.15244     3.53468     0.89923
B     -0.70215    -0.93319    -0.34330
C     -1.68230    -0.38061    -1.54479
C     -1.51286    -1.41170     1.00658
C     -1.84070    -0.32848     1.99862
C     -2.79828     0.55694    -1.17025
C     -3.04934    -0.03445     2.49844
C     -4.09906     0.36388    -1.43249
H      3.16320     1.24680    -1.93836
H      0.93538     0.28844    -2.07741
H      0.90169    -1.09393     1.74950
H      2.48794     0.84208     1.97966
H      3.35893    -0.66597     1.81052
H      4.48093     0.73538     0.07828
H     -0.52771     2.06275    -1.26305
H      0.96909     2.67824    -1.94683
H      2.70257    -1.98537    -0.63159
H      2.69769    -2.88974     0.96427
H      0.46256    -3.73587     0.54618
H     -0.87194    -3.08169    -1.37189
H      0.48587    -2.08346    -2.04635
H      1.84005     3.07061     0.45520
H      0.09489     4.12617     1.77666
H     -1.20770     3.44767     0.64915
H     -2.14386    -1.25862    -2.01644
H     -1.08784     0.08877    -2.34239
H     -2.44306    -1.90881     0.69779
H     -0.93736    -2.17984     1.54349
H     -0.99508     0.26436     2.35352
H     -2.52337     1.46932    -0.63984
H     -3.18722     0.76486     3.22260
H     -3.94209    -0.57504     2.18913
H     -4.85555     1.08391    -1.13030
H     -4.44926    -0.52749    -1.95089
45
bora-aza-Cope_TS-trans-2-conf38 E=-743.016205921 G=-742.700473 Imag-freq=1
C      2.80807    -0.51294    -0.95952
C      1.48343     0.21179    -0.96474
N      0.49572    -0.29810     0.03271
C      0.91973    -1.20237     0.94896
C      2.38700    -1.33540     1.30649
C      3.26123    -1.19229     0.09501
C      1.73116     1.74468    -0.81511
C      0.55987    -3.06845     0.08984
C     -0.74867    -2.86861    -0.34522
C     -1.09814    -1.89384    -1.30793
C      2.44128     2.16788     0.44307
C      2.03634     3.14561     1.26208
B     -1.00460    -0.26486    -0.31249
C     -1.52692     0.82533    -1.41305
C     -2.00150    -0.41545     0.98940
C     -3.44669    -0.66790     0.66589
C     -1.86017     2.25341    -1.03787
C     -4.49341     0.09541     1.01203
C     -1.61829     2.90545     0.10651
H      3.41137    -0.39515    -1.85694
H      1.03554     0.07829    -1.95503
H      0.24873    -1.34775     1.78572
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H      2.55044    -2.29383     1.80814
H      2.63169    -0.56266     2.05258
H      4.24198    -1.66056     0.08997
H      0.78209     2.27576    -0.90657
H      2.34573     2.03298    -1.68099
H      1.37458    -2.95269    -0.61922
H      0.74414    -3.77863     0.89252
H     -1.55082    -3.27739     0.26955
H     -2.12870    -1.90644    -1.66003
H     -0.38378    -1.71878    -2.11398
H      3.37187     1.64809     0.66968
H      2.61446     3.42367     2.13941
H      1.12004     3.70198     1.08064
H     -2.45832     0.40953    -1.82875
H     -0.86645     0.87333    -2.29420
H     -1.67524    -1.24546     1.63097
H     -1.93134     0.48922     1.60781
H     -3.65684    -1.57777     0.09914
H     -2.36642     2.81683    -1.82680
H     -5.50971    -0.17224     0.73351
H     -4.36590     1.01500     1.58007
H     -1.91498     3.94403     0.23293
H     -1.11720     2.43770     0.94823
45
bora-aza-Cope_TS-trans-2-conf39 E=-743.021898813 G=-742.705843 Imag-freq=1
C      2.85450    -0.46623    -1.05468
C      1.56798     0.31748    -0.95020
N      0.57403    -0.24624     0.00783
C      0.95850    -1.28082     0.79804
C      2.42133    -1.54230     1.10040
C      3.28431    -1.29372    -0.10118
C      1.90295     1.80880    -0.63237
C      0.45031    -2.98923    -0.24355
C     -0.86572    -2.66000    -0.56464
C     -1.20507    -1.56766    -1.39783
C      2.56115     2.05039     0.69878
C      2.12958     2.91809     1.62107
B     -0.93493    -0.09002    -0.27485
C     -1.40186     1.18208    -1.21060
C     -1.87976    -0.25080     1.06308
C     -3.34903    -0.37337     0.78492
C     -1.69107     2.46462    -0.47649
C     -4.13828    -1.39910     1.13859
C     -2.84277     3.15046    -0.50789
H      3.45240    -0.26840    -1.94157
H      1.10110     0.31822    -1.94147
H      0.30205    -1.47437     1.63628
H      2.53600    -2.56485     1.47203
H      2.72191    -0.88736     1.93361
H      4.23972    -1.80524    -0.18315
H      0.99895     2.41438    -0.71579
H      2.57885     2.14373    -1.43271
H      1.22722    -2.84740    -0.99007
H      0.63084    -3.79836     0.46027
H     -1.65641    -3.07007     0.06351
H     -2.25891    -1.47554    -1.65822
H     -0.54151    -1.36626    -2.24104
H      3.46996     1.48268     0.89707
H      2.66419     3.06451     2.55573
H      1.23268     3.51572     1.47219
H     -2.31249     0.89343    -1.75186
H     -0.65729     1.38436    -1.99361
H     -1.58882    -1.08718     1.70905
H     -1.71716     0.66621     1.65407
H     -3.80355     0.45162     0.23527
H     -0.89145     2.86234     0.15027
H     -5.19495    -1.41977     0.88355
H     -3.75212    -2.25218     1.69452
H     -2.97647     4.06657     0.06199
H     -3.69067     2.81492    -1.10298
45
bora-aza-Cope_TS-trans-2-conf3 E=-743.020979021 G=-742.704733 Imag-freq=1
C      1.94080     1.78165    -1.13258
C      0.58350     1.12302    -1.09274
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N      0.48557    -0.03160    -0.15853
C      1.52757    -0.29005     0.66963
C      2.52621     0.79290     1.03162
C      2.83103     1.67380    -0.14497
C     -0.51245     2.19051    -0.78695
C      2.73245    -1.61185    -0.36392
C      1.76273    -2.56155    -0.67919
C      0.65814    -2.28532    -1.51761
C     -0.36148     2.91588     0.52298
C     -1.30545     2.98374     1.46869
B     -0.47752    -1.18480    -0.45735
C     -1.72927    -0.92145    -1.49884
C     -0.91549    -2.07369     0.86162
C     -1.46388    -1.27772     2.01225
C     -3.06160    -0.51372    -0.93150
C     -0.99074    -1.27930     3.26787
C     -3.82456     0.51500    -1.32983
H      2.13404     2.40870    -2.00013
H      0.36578     0.74640    -2.09866
H      1.29156    -0.96346     1.48406
H      3.43340     0.33204     1.43321
H      2.10214     1.38705     1.85658
H      3.78160     2.19968    -0.17973
H     -1.49488     1.71743    -0.83413
H     -0.46563     2.92076    -1.60835
H      3.01978    -0.87747    -1.11138
H      3.51389    -1.87679     0.34434
H      1.70002    -3.44156    -0.03921
H      0.01544    -3.13216    -1.75746
H      0.84282    -1.63964    -2.37825
H      0.58309     3.43483     0.68469
H     -1.14949     3.54293     2.38747
H     -2.26487     2.48396     1.35412
H     -1.89260    -1.90594    -1.96503
H     -1.46970    -0.25014    -2.32754
H     -1.69461    -2.77023     0.51220
H     -0.10533    -2.70918     1.23870
H     -2.31111    -0.62637     1.79374
H     -3.45448    -1.15063    -0.13773
H     -1.43005    -0.65774     4.04408
H     -0.14765    -1.90404     3.55954
H     -4.78844     0.71924    -0.87045
H     -3.51120     1.18640    -2.12739
45
bora-aza-Cope_TS-trans-2-conf40 E=-743.020559285 G=-742.706406 Imag-freq=1
C     -2.80210    -0.14433     0.32804
C     -1.40476     0.41693     0.42487
N     -0.33804    -0.48712    -0.09023
C     -0.70625    -1.62128    -0.73254
C     -2.07486    -1.75484    -1.37007
C     -3.13670    -1.11161    -0.52746
C     -1.33882     1.77877    -0.33062
C     -0.79056    -3.07643     0.74720
C      0.48568    -2.88556     1.27155
C      0.88808    -1.68779     1.90958
C     -2.17558     2.85722     0.30243
C     -3.13844     3.55006    -0.31517
B      1.08079    -0.43117     0.50142
C      1.51952     0.92037     1.33679
C      2.24927    -0.99456    -0.51123
C      2.27812    -0.36584    -1.87825
C      2.27515     1.99654     0.60520
C      3.32079     0.23632    -2.46754
C      3.48403     2.46707     0.94502
H     -3.54907     0.33237     0.95685
H     -1.18966     0.61047     1.48195
H      0.08698    -2.09866    -1.29386
H     -2.29075    -2.81206    -1.54983
H     -2.03457    -1.28592    -2.36662
H     -4.16261    -1.45958    -0.61419
H     -1.64281     1.61972    -1.37134
H     -0.29383     2.10308    -0.34391
H     -1.64431    -2.62204     1.24242
H     -1.00517    -3.99682     0.20951
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H      1.26997    -3.56249     0.93247
H      1.88086    -1.69703     2.35909
H      0.14581    -1.19620     2.54148
H     -1.94929     3.08457     1.34576
H     -3.69215     4.33275     0.19601
H     -3.40097     3.35940    -1.35378
H      2.15537     0.59245     2.17015
H      0.64287     1.38106     1.81503
H      3.22784    -0.85678    -0.03099
H      2.14242    -2.08006    -0.65189
H      1.34722    -0.42074    -2.44694
H      1.79728     2.43064    -0.27419
H      3.24434     0.65792    -3.46691
H      4.28081     0.33757    -1.96486
H      3.97525     3.24818     0.37006
H      4.02503     2.07769     1.80620
45
bora-aza-Cope_TS-trans-2-conf41 E=-743.024767737 G=-742.716531 Imag-freq=1
C      2.67808    -0.42673    -0.74815
C      1.42087     0.36895    -0.49381
N      0.28825    -0.43002     0.05005
C      0.52009    -1.70560     0.44965
C      1.92109    -2.16856     0.80192
C      2.94239    -1.57690    -0.12521
C      1.73743     1.54786     0.47840
C      0.08129    -2.86628    -1.17774
C     -1.19701    -2.37096    -1.43635
C     -1.43417    -1.03614    -1.84241
C      2.64993     2.58542    -0.11693
C      3.81392     2.98389     0.40768
B     -1.16355    -0.04720    -0.26574
C     -1.41097     1.51875    -0.71164
C     -2.26163    -0.56237     0.84591
C     -2.09255     0.07544     2.19327
C     -2.76903     1.82506    -1.27483
C     -1.85238    -0.56048     3.35067
C     -3.71792     2.57461    -0.69510
H      3.39665     0.02165    -1.42884
H      1.09691     0.80286    -1.44640
H     -0.24967    -2.11591     1.09125
H      1.95663    -3.26189     0.79473
H      2.12688    -1.87064     1.84256
H      3.87798    -2.10551    -0.28796
H      2.17178     1.13969     1.39789
H      0.78866     2.02314     0.74887
H      0.91696    -2.50200    -1.76963
H      0.18504    -3.88746    -0.81855
H     -2.04154    -2.93387    -1.03906
H     -2.46429    -0.79206    -2.09877
H     -0.71396    -0.60062    -2.53726
H      2.30487     3.04663    -1.04413
H      4.41557     3.75554    -0.06473
H      4.20059     2.55381     1.32940
H     -0.66647     1.82748    -1.45885
H     -1.25518     2.16480     0.16398
H     -3.24774    -0.28222     0.44633
H     -2.28502    -1.65198     0.96767
H     -2.15146     1.16542     2.21905
H     -2.99527     1.39308    -2.25132
H     -1.71680    -0.01774     4.28288
H     -1.78463    -1.64614     3.40180
H     -4.68144     2.74141    -1.16991
H     -3.56155     3.04288     0.27530
45
bora-aza-Cope_TS-trans-2-conf4 E=-743.024541793 G=-742.709871 Imag-freq=1
C      2.38509    -0.85810    -1.49847
C      1.09238    -0.09466    -1.34128
N      0.43797    -0.25630    -0.01345
C      1.10623    -0.91529     0.96705
C      2.61675    -1.04834     0.93319
C      3.11874    -1.27016    -0.46344
C      1.33143     1.40896    -1.69025
C      0.51731    -2.88035     0.81159
C     -0.86431    -2.68789     0.77944
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C     -1.51655    -1.98933    -0.26373
C      2.30049     2.13368    -0.79654
C      2.03754     3.27924    -0.15776
B     -1.09482    -0.19861     0.09491
C     -1.86210     0.65010    -1.08912
C     -1.66459     0.15843     1.59755
C     -1.45713     1.58595     2.01231
C     -3.36102     0.57526    -1.06661
C     -0.77006     2.00886     3.08441
C     -4.14205     0.05357    -2.02395
H      2.72072    -1.00766    -2.52226
H      0.39257    -0.46993    -2.09661
H      0.70401    -0.76246     1.96070
H      2.92479    -1.85666     1.60298
H      3.05123    -0.12870     1.35637
H      4.06924    -1.77657    -0.60981
H      0.37596     1.93778    -1.70445
H      1.71508     1.42205    -2.72103
H      1.04900    -3.04133    -0.12260
H      0.95710    -3.36670     1.67922
H     -1.41213    -2.82598     1.71159
H     -2.60581    -1.98551    -0.24307
H     -1.11736    -2.13136    -1.27004
H      3.29035     1.68935    -0.69483
H      2.78638     3.77176     0.45673
H      1.06590     3.76363    -0.23000
H     -1.51943     0.36038    -2.09050
H     -1.58500     1.70795    -0.96072
H     -2.74605    -0.04527     1.57175
H     -1.26616    -0.49718     2.38102
H     -1.89847     2.34613     1.36447
H     -3.85260     0.98802    -0.18390
H     -0.64812     3.06661     3.30355
H     -0.30571     1.30827     3.77667
H     -5.22460     0.03227    -1.92780
H     -3.72144    -0.37141    -2.93392
45
bora-aza-Cope_TS-trans-2-conf5 E=-743.024768613 G=-742.710750 Imag-freq=1
C      2.77779    -0.30123    -0.60944
C      1.43795     0.37961    -0.47514
N      0.38326    -0.45559     0.16271
C      0.73784    -1.63982     0.72182
C      2.17106    -1.90535     1.14196
C      3.14703    -1.32702     0.15971
C      1.60257     1.70548     0.33053
C      0.45702    -3.04091    -0.74825
C     -0.85879    -2.71880    -1.08068
C     -1.22939    -1.47575    -1.64810
C      2.41963     2.74472    -0.38778
C      3.52166     3.32996     0.09369
B     -1.09372    -0.26310    -0.22001
C     -1.48621     1.20789    -0.84806
C     -2.15243    -0.72467     0.95182
C     -1.99154     0.03831     2.23514
C     -2.79074     1.27418    -1.58888
C     -2.87796     0.88166     2.78535
C     -3.90282     1.91022    -1.19242
H      3.46158     0.13211    -1.33422
H      1.08890     0.64149    -1.48047
H      0.00269    -2.05080     1.40296
H      2.31948    -2.98165     1.26906
H      2.32070    -1.46441     2.14067
H      4.13760    -1.76669     0.07818
H      2.05034     1.47261     1.30320
H      0.60179     2.10821     0.51983
H      1.26697    -2.66789    -1.36962
H      0.65406    -3.99261    -0.26031
H     -1.64872    -3.32180    -0.63273
H     -2.27150    -1.38848    -1.95342
H     -0.53982    -1.04888    -2.37934
H      2.05501     3.03877    -1.37371
H      4.05403     4.09059    -0.47076
H      3.92450     3.06989     1.07049
H     -0.70658     1.56079    -1.53696
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H     -1.52379     1.92991    -0.02007
H     -3.17208    -0.58324     0.57020
H     -2.05990    -1.79708     1.17391
H     -1.04163    -0.10361     2.75604
H     -2.82360     0.75506    -2.54852
H     -2.66472     1.40828     3.71237
H     -3.84390     1.07508     2.32227
H     -4.80773     1.90374    -1.79487
H     -3.94387     2.45440    -0.25070
45
bora-aza-Cope_TS-trans-2-conf6 E=-743.024108450 G=-742.709726 Imag-freq=1
C      2.64573    -0.24773    -1.39532
C      1.21464     0.22289    -1.30008
N      0.49477    -0.23441    -0.07997
C      1.19304    -0.88650     0.88454
C      2.69635    -0.72483     1.00784
C      3.35408    -0.64924    -0.33873
C      1.16931     1.77694    -1.45140
C      1.03172    -2.87863     0.42475
C     -0.35431    -2.95227     0.28374
C     -1.06403    -2.25362    -0.72155
C      1.88301     2.55206    -0.37762
C      1.33249     3.53252     0.34706
B     -1.02283    -0.46782    -0.12206
C     -1.84534     0.38741    -1.26400
C     -1.76776    -0.42054     1.34341
C     -1.75814     0.93296     1.99076
C     -3.27664    -0.01561    -1.47359
C     -1.24561     1.23457     3.19383
C     -4.35900     0.72475    -1.19306
H      3.09456    -0.18664    -2.38426
H      0.67604    -0.17884    -2.16647
H      0.68105    -0.94847     1.83681
H      3.10233    -1.54560     1.60647
H      2.89554     0.19184     1.58532
H      4.39788    -0.93685    -0.43420
H      0.13093     2.10828    -1.51682
H      1.63386     1.99910    -2.42333
H      1.64964    -2.80021    -0.46592
H      1.49832    -3.39227     1.26210
H     -0.92499    -3.32445     1.13441
H     -2.12868    -2.47371    -0.79020
H     -0.58438    -2.18294    -1.69979
H      2.92948     2.29770    -0.21074
H      1.90417     4.07649     1.09420
H      0.29277     3.82515     0.21569
H     -1.33771     0.31277    -2.23655
H     -1.82951     1.45088    -0.98785
H     -2.81306    -0.70700     1.15224
H     -1.38200    -1.15777     2.05786
H     -2.19956     1.74599     1.41120
H     -3.44138    -1.00631    -1.90112
H     -1.26033     2.24961     3.58287
H     -0.79371     0.47359     3.82839
H     -5.36500     0.35402    -1.37246
H     -4.27270     1.72479    -0.77129
45
bora-aza-Cope_TS-trans-2-conf7 E=-743.020559373 G=-742.706403 Imag-freq=1
C     -2.80204    -0.14386     0.32820
C     -1.40457     0.41705     0.42510
N     -0.33807    -0.48710    -0.09026
C     -0.70654    -1.62119    -0.73258
C     -2.07521    -1.75447    -1.37004
C     -3.13688    -1.11100    -0.52737
C     -1.33834     1.77904    -0.33009
C     -0.79101    -3.07629     0.74717
C      0.48544    -2.88584     1.27122
C      0.88828    -1.68825     1.90927
C     -2.17523     2.85743     0.30290
C     -3.13782     3.55048    -0.31488
B      1.08082    -0.43151     0.50124
C      1.51989     0.91983     1.33679
C      2.24909    -0.99487    -0.51169
C      2.27750    -0.36607    -1.87868
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C      2.27571     1.99592     0.60530
C      3.31961     0.23722    -2.46783
C      3.48470     2.46613     0.94517
H     -3.54890     0.33300     0.95699
H     -1.18938     0.61029     1.48223
H      0.08656    -2.09870    -1.29396
H     -2.29134    -2.81165    -1.54976
H     -2.03488    -1.28558    -2.36660
H     -4.16288    -1.45866    -0.61416
H     -1.64200     1.62020    -1.37093
H     -0.29333     2.10331    -0.34298
H     -1.64447    -2.62160     1.24260
H     -1.00607    -3.99660     0.20953
H      1.26945    -3.56293     0.93185
H      1.88119    -1.69771     2.35849
H      0.14626    -1.19660     2.54142
H     -1.94924     3.08458     1.34634
H     -3.69163     4.33312     0.19627
H     -3.40004     3.36003    -1.35361
H      2.15577     0.59168     2.17003
H      0.64336     1.38058     1.81520
H      3.22775    -0.85701    -0.03169
H      2.14225    -2.08037    -0.65234
H      1.34672    -0.42186    -2.44749
H      1.79785     2.43032    -0.27395
H      3.24279     0.65882    -3.46717
H      4.27948     0.33939    -1.96509
H      3.97607     3.24725     0.37035
H      4.02564     2.07645     1.80626
45
bora-aza-Cope_TS-trans-2-conf8 E=-743.019659635 G=-742.704731 Imag-freq=1
C      2.91655    -0.05641    -1.02508
C      1.50704     0.48067    -0.95085
N      0.62642    -0.21915     0.02958
C      1.19360    -1.12741     0.86312
C      2.67692    -1.09615     1.17634
C      3.48730    -0.74571    -0.03640
C      1.56223     2.01956    -0.69498
C      1.02828    -2.94692    -0.10642
C     -0.31840    -2.88537    -0.46127
C     -0.83661    -1.90671    -1.34219
C      2.14825     2.43067     0.62830
C      1.55272     3.23775     1.51358
B     -0.88363    -0.35781    -0.26451
C     -1.56698     0.75913    -1.25500
C     -1.79905    -0.65146     1.07055
C     -3.17480    -1.20078     0.81715
C     -2.04604     2.02909    -0.59848
C     -4.34095    -0.65395     1.18864
C     -3.26168     2.57703    -0.73333
H      3.47172     0.20865    -1.92208
H      1.05388     0.35687    -1.94041
H      0.57953    -1.40945     1.70825
H      2.97750    -2.06130     1.59475
H      2.84282    -0.35931     1.97825
H      4.52131    -1.07468    -0.09739
H      0.56552     2.44764    -0.81109
H      2.17789     2.43747    -1.50478
H      1.78073    -2.69137    -0.84743
H      1.34163    -3.67854     0.63455
H     -1.02847    -3.42176     0.16873
H     -1.87658    -2.02733    -1.64284
H     -0.19558    -1.60551    -2.17263
H      3.14428     2.04988     0.85292
H      2.04021     3.51643     2.44393
H      0.56216     3.65192     1.33789
H     -2.43168     0.29304    -1.74581
H     -0.88353     1.02594    -2.07482
H     -1.30047    -1.36384     1.74241
H     -1.89101     0.28560     1.63965
H     -3.21717    -2.15658     0.29045
H     -1.33704     2.54674     0.04902
H     -5.29065    -1.13442     0.96633
H     -4.38296     0.29473     1.71982
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H     -3.53084     3.49910    -0.22385
H     -4.03026     2.11505    -1.35062
45
bora-aza-Cope_TS-trans-2-conf9 E=-743.019387702 G=-742.703782 Imag-freq=1
C      2.69139     0.85325    -1.04085
C      1.18887     0.72158    -1.10318
N      0.60022    -0.16422    -0.05952
C      1.41668    -0.65639     0.90374
C      2.71670     0.03307     1.26710
C      3.40539     0.58165     0.05233
C      0.54628     2.14341    -1.08413
C      2.11709    -2.46328     0.15008
C      0.88596    -3.03134    -0.16849
C      0.01794    -2.49455    -1.14875
C      0.79834     2.94770     0.16229
C     -0.15141     3.53469     0.89905
B     -0.70237    -0.93305    -0.34322
C     -1.68233    -0.38051    -1.54491
C     -1.51320    -1.41099     1.00678
C     -1.84070    -0.32739     1.99852
C     -2.79838     0.55703    -1.17060
C     -3.04916    -0.03311     2.49861
C     -4.09920     0.36358    -1.43237
H      3.16341     1.24582    -1.93873
H      0.93533     0.28810    -2.07754
H      0.90145    -1.09370     1.74963
H      3.35878    -0.66625     1.81056
H      2.48810     0.84203     1.97935
H      4.48109     0.73442     0.07797
H     -0.52735     2.06273    -1.26306
H      0.96944     2.67784    -1.94724
H      2.70208    -1.98606    -0.63131
H      2.69712    -2.89002     0.96478
H      0.46175    -3.73573     0.54708
H     -0.87270    -3.08182    -1.37112
H      0.48529    -2.08413    -2.04600
H      1.84094     3.07054     0.45447
H      0.09619     4.12626     1.77635
H     -1.20674     3.44766     0.64929
H     -2.14381    -1.25854    -2.01662
H     -1.08773     0.08886    -2.34241
H     -2.44355    -1.90793     0.69816
H     -0.93788    -2.17913     1.54387
H     -0.99493     0.26553     2.35293
H     -2.52349     1.46979    -0.64083
H     -3.18677     0.76647     3.22252
H     -3.94204    -0.57376     2.18979
H     -4.85574     1.08363    -1.13035
H     -4.44938    -0.52814    -1.95016
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TS_trans-6:

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45
bora-aza-Cope_TS-trans-6-conf10 E=-743.024637603 G=-742.711313 Imag-freq=1
C     -2.48813    -1.13068    -1.09447
C     -1.01791    -1.09344    -0.96554
N     -0.42113    -0.33702     0.00394
C     -1.26079     0.16548     1.12939
C     -2.61426    -0.56369     1.28022
C     -3.26635    -0.86603    -0.03817
C     -0.62529    -3.03917    -0.45794
C     -1.43564     1.70613     1.03590
C     -2.25260     2.22234    -0.11666
C     -3.30444     3.04143     0.00030
C      0.76265    -2.94186    -0.29354
C      1.36264    -2.17779     0.72253
B      1.09626    -0.34689     0.09006
C      1.76823     0.59189     1.25631
C      1.87539    -0.22335    -1.34872
C      1.60555     1.07789    -2.04996
C      3.20178     0.30049     1.59792
C      2.49711     2.04070    -2.32748
C      4.25657     1.09085     1.35244
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H     -2.89358     -1.40833     -2.06283
H     -0.48102     -1.12580     -1.90496
H     -0.70326     -0.01801      2.05059
H     -3.26797      0.04545      1.91313
H     -2.46306     -1.50612      1.82705
H     -4.35008     -0.89792     -0.10852
H     -1.01539     -3.61708     -1.29219
H     -1.25737     -3.03941      0.42538
H     -0.43388      2.14764      0.97881
H     -1.87717      2.04819      1.98043
H     -1.92718      1.92155     -1.11191
H     -3.83970      3.40797     -0.87146
H     -3.66450      3.37236      0.97264
H      1.38651     -3.23420     -1.13803
H      2.44633     -2.23476      0.80305
H      0.85313     -2.12658      1.68526
H      1.19325      0.52602      2.19043
H      1.70107      1.63767      0.92363
H      1.59846     -1.04260     -2.02608
H      2.95417     -0.32659     -1.17498
H      0.56814      1.25054     -2.34553
H      3.39060     -0.64636      2.10683
H      2.20465      2.96181     -2.82562
H      3.54736      1.93921     -2.06026
H      5.26437      0.79935      1.63733
H      4.14564      2.05241      0.85474
45
bora-aza-Cope_TS-trans-6-conf11 E=-743.017075397 G=-742.701471 Imag-freq=1
C     -1.08986     -2.67393     -1.32719
C     -0.00025     -1.91348     -0.68680
N     -0.17440     -0.61150     -0.30519
C     -1.61072     -0.34418      0.04552
C     -2.50082     -0.67654     -1.16331
C     -2.25305     -2.08060     -1.62814
C      0.31297     -2.92824      1.09197
C     -1.92232      1.05165      0.60515
C     -3.37066      1.20329      0.99569
C     -4.17328      2.19998      0.60722
C      1.34387     -2.13608      1.60670
C      1.17610     -0.77694      1.95749
B      1.08352      0.07978      0.24703
C      1.11477      1.68282      0.59916
C      2.44509     -0.31299     -0.61449
C      3.73556      0.25452     -0.09526
C      1.06191      2.59690     -0.59392
C      4.58183      1.05607     -0.75762
C      0.28847      3.68324     -0.73903
H     -0.86476     -3.69354     -1.62511
H      0.96923     -2.14394     -1.10447
H     -1.87749     -1.06643      0.83550
H     -2.32921      0.04297     -1.97981
H     -3.54854     -0.55848     -0.86963
H     -3.01414     -2.59682     -2.20796
H      0.53559     -3.94845      0.78935
H     -0.70193     -2.77320      1.45069
H     -1.64103      1.82751     -0.11172
H     -1.32709      1.20418      1.50895
H     -3.76341      0.44692      1.67803
H     -5.19943      2.27137      0.95719
H     -3.82919      2.97807     -0.07103
H      2.36318     -2.49847      1.47381
H      2.02489     -0.28778      2.43473
H      0.22142     -0.49458      2.40186
H      2.10516      1.82061      1.05930
H      0.39967      2.02137      1.35280
H      2.30516      0.01484     -1.65623
H      2.59407     -1.39912     -0.66161
H      4.00667     -0.03455      0.92303
H      1.73654      2.34640     -1.41378
H      5.50139      1.41525     -0.30238
H      4.37868      1.38240     -1.77625
H      0.32431      4.28984     -1.64058
H     -0.40418      4.00239      0.03769
45
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bora-aza-Cope_TS-trans-6-conf12 E=-743.015769443 G=-742.699731 Imag-freq=1
C 0.67034 -2.68628 -0.95772
C 1.04374 -1.50298 -0.16282
N 0.21777 -0.41860 -0.07404
C -1.22511 -0.80922 -0.21923
C -1.42337 -1.55300 -1.55182
C -0.46057 -2.69657 -1.67545
C 1.12021 -2.25981 1.77178
C -2.23015 0.34323 -0.04828
C -3.66276 -0.06434 -0.29214
C -4.59038 -0.17186 0.66616
C 1.56875 -1.09250 2.39174
C 0.80124 0.09227 2.46298
B 0.83166 0.77728 0.66939
C 0.06313 2.22267 0.86812
C 2.42116 1.04661 0.26267
C 2.71606 1.12318 -1.21042
C -0.01759 3.14105 -0.32007
C 3.62792 0.39572 -1.87327
C -1.11792 3.74255 -0.79678
H 1.39261 -3.49572 -1.00171
H 2.09689 -1.26930 -0.21781
H -1.43936 -1.53725 0.58006
H -1.31838 -0.86198 -2.40350
H -2.44754 -1.93611 -1.59061
H -0.68863 -3.51496 -2.35370
H 1.79111 -3.11229 1.70286
H 0.06346 -2.51345 1.80968
H -1.96312 1.15624 -0.73162
H -2.15997 0.72772 0.96952
H -3.95556 -0.25694 -1.32362
H -5.61472 -0.45271 0.43711
H -4.35537 0.02081 1.71124
H 2.63995 -1.01014 2.57500
H 1.22838 0.91012 3.04288
H -0.27138 -0.02522 2.62078
H 0.70391 2.72942 1.60715
H -0.91963 2.15734 1.34178
H 3.11775 0.32941 0.71344
H 2.67924 2.01751 0.71349
H 2.12034 1.82806 -1.79156
H 0.92569 3.35605 -0.82315
H 3.77204 0.50161 -2.94555
H 4.26176 -0.32855 -1.36349
H -1.07470 4.40445 -1.65807
H -2.09566 3.59541 -0.34196
45
bora-aza-Cope_TS-trans-6-conf13 E=-743.012508222 G=-742.696970 Imag-freq=1
C -0.71216 -2.63365 1.20315
C -1.17621 -1.47264 0.42525
N -0.32568 -0.46519 0.07611
C 1.08442 -0.96001 -0.06339
C 1.52547 -1.63130 1.24822
C 0.54659 -2.69028 1.66016
C -1.71846 -2.33709 -1.41077
C 2.11141 0.08220 -0.53012
C 3.49311 -0.49935 -0.68892
C 4.60848 0.00542 -0.15069
C -2.18896 -1.17322 -2.02022
C -1.36411 -0.06795 -2.32841
B -1.00211 0.73352 -0.60105
C -0.20165 2.10237 -1.04752
C -2.46533 1.12940 0.04723
C -2.61477 1.43987 1.52221
C 0.20952 3.04925 0.04623
C -1.70244 1.34270 2.49863
C 1.41451 3.61958 0.19679
H -1.45680 -3.38051 1.46105
H -2.17790 -1.15678 0.67996
H 1.06366 -1.75319 -0.82932
H 1.64692 -0.88077 2.04553
H 2.51490 -2.07397 1.09684
H 0.86563 -3.48312 2.33208
H -2.42541 -3.11893 -1.14520

```
H     -0.71228    -2.68670    -1.62890
H      2.13554     0.93398     0.15520
H      1.80455     0.45688    -1.50967
H      3.56942    -1.38248    -1.32626
H      5.58106    -0.44196    -0.33646
H      4.58511     0.88391     0.49083
H     -3.26616    -1.00817    -2.00532
H     -1.83122     0.74965    -2.87684
H     -0.35190    -0.28608    -2.66962
H     -0.95880     2.63163    -1.64791
H      0.63992     1.94760    -1.72863
H     -3.24467     0.38601    -0.17910
H     -2.82364     2.01837    -0.49768
H     -3.61539     1.77217     1.81269
H     -0.56329     3.29645     0.77365
H     -1.95552     1.59167     3.52652
H     -0.68454     1.01701     2.30745
H      1.62058     4.30432     1.01590
H      2.23409     3.42008    -0.49134
45
bora-aza-Cope_TS-trans-6-conf14 E=-743.017312700 G=-742.702004 Imag-freq=1
C      2.48638    -1.87742     0.37922
C      1.04611    -1.58255     0.28303
N      0.56332    -0.34202    -0.04790
C      1.52807     0.47619    -0.86116
C      2.96561     0.42152    -0.29594
C      3.40648    -0.94412     0.11757
C      0.55095    -2.82984    -1.27045
C      1.17666     1.96973    -1.04144
C      1.15680     2.78711     0.22631
C      1.73390     3.98540     0.37043
C     -0.82466    -2.58298    -1.27738
C     -1.36290    -1.32562    -1.61764
B     -0.98539    -0.26797    -0.08871
C     -1.74646     1.14630    -0.47884
C     -1.69907    -0.98323     1.21724
C     -1.49113    -0.21556     2.49038
C     -3.24036     1.13651    -0.31274
C     -0.89752    -0.66960     3.60487
C     -4.14313     1.18566    -1.30345
H      2.75257    -2.87852     0.70469
H      0.45622    -2.10569     1.02174
H      1.54997     0.03303    -1.86968
H      3.05811     1.10440     0.56167
H      3.63424     0.82466    -1.06583
H      4.46709    -1.14421     0.24767
H      0.91078    -3.80572    -0.95488
H      1.17845    -2.32960    -2.00443
H      0.22795     2.07429    -1.56674
H      1.93589     2.38202    -1.71700
H      0.61830     2.36256     1.07275
H      1.66231     4.54121     1.30135
H      2.29374     4.45146    -0.43829
H     -1.46441    -3.28362    -0.74092
H     -2.44758    -1.25028    -1.68185
H     -0.84675    -0.76925    -2.40121
H     -1.53665     1.43402    -1.51459
H     -1.35530     1.95071     0.15878
H     -1.41104    -2.02726     1.38313
H     -2.77515    -1.01701     0.99450
H     -1.83889     0.81981     2.49132
H     -3.61771     1.09625     0.71003
H     -0.76320    -0.03626     4.47813
H     -0.52738    -1.69091     3.67879
H     -5.21131     1.17613    -1.10236
H     -3.84082     1.23670    -2.34820
45
bora-aza-Cope_TS-trans-6-conf15 E=-743.015074346 G=-742.700164 Imag-freq=1
C     -1.57189    -2.39474    -1.39571
C     -0.40382    -1.81798    -0.70567
N     -0.34194    -0.48512    -0.40733
C     -1.72412     0.07118    -0.18078
C     -2.57553    -0.15798    -1.44158
C     -2.57002    -1.60922    -1.82151
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C     -0.42232    -2.75649     1.14742
C     -1.80619     1.52726     0.31621
C     -3.22619     1.99848     0.52491
C     -3.79029     2.18225     1.72395
C      0.69368    -2.13020     1.71018
C      0.75253    -0.74228     1.97512
B      0.98618    -0.01885     0.22253
C      1.29484     1.57576     0.45514
C      2.31900    -0.71900    -0.46394
C      3.60703    -0.54166     0.29061
C      1.40241     2.37892    -0.81432
C      4.73001     0.03559    -0.15919
C      2.47432     3.06782    -1.23192
H     -1.53035    -3.45531    -1.62462
H      0.52774    -2.26140    -1.02527
H     -2.17732    -0.54280     0.61414
H     -2.21809     0.46806    -2.27446
H     -3.60305     0.15740    -1.23732
H     -3.37345    -2.00392    -2.43832
H     -0.36886    -3.81733     0.91587
H     -1.41585    -2.39806     1.40626
H     -1.31316     2.19383    -0.39847
H     -1.28364     1.61024     1.26923
H     -3.81165     2.22016    -0.36642
H     -4.81289     2.53587     1.82254
H     -3.24622     1.98795     2.64628
H      1.63579    -2.67807     1.68762
H      1.63097    -0.38211     2.50956
H     -0.16870    -0.26403     2.30791
H      2.25798     1.63494     0.97771
H      0.57161     2.05812     1.11976
H      2.43935    -0.30134    -1.47483
H      2.20187    -1.80203    -0.59646
H      3.62441    -0.94789     1.30463
H      0.52180     2.38858    -1.45949
H      5.62093     0.10604     0.46009
H      4.79143     0.46251    -1.15821
H      2.46697     3.61674    -2.17054
H      3.39443     3.09774    -0.65202
45
bora-aza-Cope_TS-trans-6-conf16 E=-743.017075374 G=-742.701470 Imag-freq=1
C     -1.08989    -2.67384    -1.32730
C     -0.00026    -1.91352    -0.68677
N     -0.17438    -0.61152    -0.30508
C     -1.61072    -0.34411     0.04546
C     -2.50072    -0.67634    -1.16349
C     -2.25298    -2.08038    -1.62841
C      0.31282    -2.92831     1.09186
C     -1.92233     1.05170     0.60515
C     -3.37070     1.20332     0.99559
C     -4.17323     2.20015     0.60730
C      1.34378    -2.13631     1.60679
C      1.17627    -0.77721     1.95769
B      1.08349     0.07964     0.24724
C      1.11474     1.68267     0.59943
C      2.44503    -0.31309    -0.61433
C      3.73546     0.25479    -0.09540
C      1.06211     2.59674    -0.59368
C      4.58152     1.05631    -0.75806
C      0.28872     3.68309    -0.73898
H     -0.86486    -3.69346    -1.62523
H      0.96923    -2.14398    -1.10444
H     -1.87763    -1.06639     0.83536
H     -2.32900     0.04323    -1.97991
H     -3.54846    -0.55827    -0.86990
H     -3.01403    -2.59650    -2.20836
H      0.53542    -3.94852     0.78922
H     -0.70208    -2.77327     1.45057
H     -1.64100     1.82760    -0.11165
H     -1.32716     1.20418     1.50900
H     -3.76356     0.44679     1.67771
H     -5.19940     2.27152     0.95720
H     -3.82903     2.97839    -0.07073
H      2.36305    -2.49888     1.47406
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H      2.02512    -0.28837     2.43513
H      0.22161    -0.49468     2.40200
H      2.10503     1.82046     1.05978
H      0.39948     2.02122     1.35291
H      2.30492     0.01438    -1.65616
H      2.59420    -1.39921    -0.66111
H      4.00674    -0.03398     0.92293
H      1.73687     2.34619    -1.41343
H      5.50107     1.41576    -0.30301
H      4.37820     1.38234    -1.77675
H      0.32474     4.28965    -1.64055
H     -0.40407     4.00230     0.03759
45
bora-aza-Cope_TS-trans-6-conf17 E=-743.024637693 G=-742.711387 Imag-freq=1
C      2.48850    -1.13007     1.09416
C      1.01826    -1.09327     0.96530
N      0.42119    -0.33704    -0.00416
C      1.26082     0.16603    -1.12940
C      2.61435    -0.56294    -1.28050
C      3.26660    -0.86515     0.03783
C      0.62626    -3.03919     0.45775
C      1.43557     1.70667    -1.03547
C      2.25213     2.22276     0.11742
C      3.30372     3.04225     0.00094
C     -0.76170    -2.94234     0.29324
C     -1.36187    -2.17852    -0.72290
B     -1.09618    -0.34742    -0.09031
C     -1.76832     0.59097    -1.25673
C     -1.87533    -0.22433     1.34847
C     -1.60637     1.07711     2.04970
C     -3.20233     0.30039    -1.59713
C     -2.49885     2.03871     2.32844
C     -4.25606     1.09266    -1.35327
H      2.89408    -1.40765     2.06249
H      0.48142    -1.12587     1.90474
H      0.70327    -0.01715    -2.05066
H      3.26787     0.04626    -1.91353
H      2.46317    -1.50540    -1.82729
H      4.35034    -0.89679     0.10812
H      1.01646    -3.61692     1.29209
H      1.25843    -3.03930    -0.42550
H      0.43377     2.14812    -0.97862
H      1.87736     2.04894    -1.97980
H      1.92659     1.92158     1.11251
H      3.83866     3.40871     0.87293
H      3.66389     3.37358    -0.97122
H     -1.38554    -3.23487     1.13768
H     -2.44552    -2.23588    -0.80351
H     -0.85226    -2.12707    -1.68556
H     -1.19401     0.52379    -2.19120
H     -1.70017     1.63703    -0.92514
H     -1.59773    -1.04335     2.02584
H     -2.95406    -0.32837     1.17490
H     -0.56888     1.25094     2.34430
H     -3.39250    -0.64744    -2.10368
H     -2.20703     2.96003     2.82657
H     -3.54925     1.93600     2.06224
H     -5.26431     0.80173    -1.63714
H     -4.14379     2.05530    -0.85794
45
bora-aza-Cope_TS-trans-6-conf18 E=-743.013421599 G=-742.697855 Imag-freq=1
C     -1.56635    -2.65092    -1.09653
C     -0.41937    -1.89052    -0.56903
N     -0.44631    -0.52719    -0.44289
C     -1.85195    -0.02243    -0.23377
C     -2.77095    -0.53975    -1.35877
C     -2.66412    -2.02235    -1.53324
C     -0.27614    -2.60877     1.36419
C     -2.06261     1.50824    -0.10915
C     -2.19917     2.01119     1.30555
C     -3.24263     2.71494     1.75938
C      0.85699    -1.88788     1.74796
C      0.87176    -0.47915     1.86325
B      0.88395     0.08962     0.05507
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C      1.07147     1.71651     0.16396
C      2.20818    -0.56833    -0.69337
C      3.53911    -0.11380    -0.16916
C      1.22687     2.42613    -1.15563
C      4.46214    -0.89233     0.41598
C      2.25954     3.19688    -1.52663
H     -1.43677    -3.72501    -1.18847
H      0.52830    -2.29706    -0.88944
H     -2.21149    -0.48304     0.70007
H     -2.54612    -0.02078    -2.30428
H     -3.80033    -0.26760    -1.09970
H     -3.46875    -2.56435    -2.02366
H     -0.19990    -3.68658     1.24522
H     -1.25835    -2.25270     1.66629
H     -2.98983     1.75678    -0.63613
H     -1.27486     2.03978    -0.64345
H     -1.39531     1.77271     2.00050
H     -3.29248     3.05449     2.79017
H     -4.07890     2.97682     1.11411
H      1.81862    -2.39660     1.68434
H      1.78655    -0.03648     2.25549
H     -0.03139    -0.01260     2.25605
H      1.97679     1.89778     0.75720
H      0.26742     2.19109     0.73353
H      2.13101    -0.25951    -1.74947
H      2.22339    -1.66305    -0.69507
H      3.76758     0.94646    -0.27584
H      0.42430     2.28476    -1.88305
H      5.40149    -0.48554     0.78203
H      4.30800    -1.96227     0.54764
H      2.29660     3.66619    -2.50654
H      3.10210     3.38265    -0.86266
45
bora-aza-Cope_TS-trans-6-conf19 E=-743.015853748 G=-742.701002 Imag-freq=1
C     -1.78284    -2.53204    -0.54784
C     -0.58151    -1.87138    -0.00845
N     -0.38289    -0.52477    -0.13445
C     -1.68716     0.22101    -0.22220
C     -2.53601    -0.35133    -1.37261
C     -2.68305    -1.83793    -1.25497
C     -0.76496    -2.19676     2.03081
C     -1.56914     1.75428    -0.33257
C     -2.90061     2.44831    -0.49534
C     -3.49634     3.16770     0.46254
C      0.45432    -1.62816     2.40458
C      0.74179    -0.25196     2.25512
B      0.99327    -0.03747     0.37695
C      1.42562     1.54294     0.21621
C      2.22883    -1.02549    -0.10005
C      2.36089    -1.13104    -1.59408
C      2.81681     1.87887     0.68119
C      3.41148    -0.75138    -2.33661
C      3.76500     2.50337    -0.03093
H     -1.84772    -3.60836    -0.42135
H      0.30873    -2.47492    -0.11186
H     -2.23678     0.01305     0.71042
H     -2.09997    -0.08068    -2.34766
H     -3.52586     0.11350    -1.33951
H     -3.51161    -2.33397    -1.75407
H     -0.89712    -3.27176     2.12287
H     -1.67756    -1.61427     2.13349
H     -0.92556     2.00744    -1.18287
H     -1.09963     2.14504     0.56919
H     -3.38660     2.37053    -1.46700
H     -4.44921     3.66146     0.29286
H     -3.04853     3.28849     1.44710
H      1.29442    -2.30633     2.55454
H      1.68697     0.08862     2.67639
H     -0.07927     0.44140     2.44109
H      0.75359     2.18689     0.79438
H      1.32825     1.85793    -0.83177
H      2.13422    -2.04030     0.31008
H      3.16547    -0.63379     0.31448
H      1.50036    -1.55164    -2.11937
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H      3.05790     1.61072     1.71210
H      3.41029    -0.85497    -3.41905
H      4.30193    -0.31859    -1.88540
H      4.74085     2.72809     0.39261
H      3.59767     2.80311    -1.06401
45
bora-aza-Cope_TS-trans-6-conf1 E=-743.025794842 G=-742.711782 Imag-freq=1
C      1.38614    -2.51938    -0.26128
C      0.10087    -1.83397    -0.01044
N      0.03509    -0.46759    -0.02224
C      1.23938     0.28538    -0.46321
C      2.11576    -0.50922    -1.44930
C      2.35631    -1.90988    -0.95606
C     -0.98684    -2.45257    -1.62383
C      2.04107     0.73301     0.79115
C      3.09289     1.76533     0.48888
C      4.39843     1.64063     0.75270
C     -2.15895    -1.71833    -1.39265
C     -2.19845    -0.31565    -1.46769
B     -1.30349     0.20840     0.17269
C     -1.34466     1.85958     0.17455
C     -2.22162    -0.39824     1.39616
C     -1.71628    -0.00012     2.75217
C     -1.32053     2.62705    -1.11730
C     -1.28394    -0.83129     3.71308
C     -2.31421     3.39354    -1.58997
H      1.47985    -3.54123     0.09430
H     -0.53971    -2.31593     0.71733
H      0.89483     1.18312    -0.97629
H      3.05832     0.02668    -1.59609
H      1.62708    -0.54353    -2.43448
H      3.29394    -2.41140    -1.17965
H     -1.01674    -3.53447    -1.51962
H     -0.28473    -2.09054    -2.36949
H      2.49268    -0.14292     1.27014
H      1.32328     1.15290     1.50624
H      2.73624     2.68667     0.02449
H      5.10393     2.43424     0.52209
H      4.80302     0.74136     1.21302
H     -2.97164    -2.22263    -0.87026
H     -3.16493     0.17186    -1.34657
H     -1.56342     0.16431    -2.21028
H     -0.51435     2.21652     0.80384
H     -2.25937     2.14872     0.70920
H     -2.32930    -1.48897     1.36332
H     -3.23423     0.01169     1.25964
H     -1.67992     1.07203     2.95605
H     -0.41811     2.55348    -1.72704
H     -0.90526    -0.45897     4.66168
H     -1.29615    -1.91191     3.58011
H     -2.22971     3.91443    -2.54025
H     -3.24594     3.52045    -1.04098
45
bora-aza-Cope_TS-trans-6-conf20 E=-743.016495899 G=-742.700671 Imag-freq=1
C     -0.84077    -2.63148     0.96742
C     -1.19222    -1.40267     0.23309
N     -0.27076    -0.41724     0.01685
C      1.12161    -0.97202    -0.04912
C      1.42743    -1.74305     1.24609
C      0.37475    -2.77745     1.51206
C     -1.64274    -2.11795    -1.66576
C      2.22781     0.04522    -0.36484
C      3.59105    -0.59203    -0.45428
C      4.68055    -0.17711     0.20090
C     -2.04409    -0.89884    -2.21439
C     -1.16668     0.19278    -2.40473
B     -0.84685     0.85094    -0.62851
C      0.04524     2.20046    -0.94621
C     -2.31475     1.29444     0.01412
C     -2.36926     1.38576     1.51465
C      0.41650     3.08411     0.21266
C     -3.24174     0.75424     2.31465
C      1.63942     3.54995     0.50738
H     -1.63522    -3.35585     1.11907
```

H -2.19188 -1.05230 0.44469
H 1.12703 -1.71419 -0.86498
H 1.51471 -1.04832 2.09689
H 2.40645 -2.22154 1.14438
H 0.60569 -3.62528 2.15219
H -2.38795 -2.89043 -1.49388
H -0.63940 -2.48855 -1.86213
H 2.23370 0.84937 0.37621
H 2.01823 0.49545 -1.33812
H 3.67940 -1.43613 -1.14101
H 5.64433 -0.65913 0.06183
H 4.64418 0.65946 0.89564
H -3.11434 -0.69371 -2.23360
H -1.58066 1.06224 -2.91492
H -0.15049 -0.04234 -2.72314
H -0.63805 2.78990 -1.57810
H 0.92857 2.03041 -1.56756
H -3.14904 0.66607 -0.32056
H -2.52638 2.29367 -0.39723
H -1.61722 2.01439 1.99288
H -0.40504 3.39645 0.85806
H -3.20583 0.86258 3.39573
H -4.02211 0.10923 1.91317
H 1.80842 4.19912 1.36285
H 2.50981 3.29916 -0.09580
45
bora-aza-Cope_TS-trans-6-conf21 E=-743.022601848 G=-742.708007 Imag-freq=1
C 2.12340 -1.81161 0.10271
C 0.70505 -1.50308 0.37465
N 0.14582 -0.34405 -0.08871
C 0.89850 0.46003 -1.09071
C 1.97296 -0.34723 -1.85086
C 2.74586 -1.27137 -0.95218
C -0.20784 -3.01327 -0.65918
C 1.46754 1.75778 -0.44942
C 2.61345 1.61456 0.51539
C 2.59371 2.02572 1.78860
C -1.54899 -2.63963 -0.48777
C -2.07931 -1.46347 -1.04114
B -1.32517 -0.09969 0.15557
C -2.01205 1.30460 -0.35463
C -1.87435 -0.48734 1.65768
C -1.51896 0.52249 2.71096
C -2.11118 1.67271 -1.80896
C -0.78109 0.29495 3.80817
C -1.72341 2.82956 -2.36575
H 2.61191 -2.51902 0.76628
H 0.34695 -1.82196 1.34505
H 0.17128 0.80084 -1.82826
H 2.63906 0.35196 -2.36775
H 1.49121 -0.93908 -2.64365
H 3.78176 -1.50632 -1.18186
H 0.14998 -3.91835 -0.17426
H 0.27503 -2.78979 -1.60618
H 0.64765 2.29039 0.04159
H 1.79351 2.38807 -1.29005
H 3.52865 1.17115 0.12477
H 3.46220 1.92210 2.43368
H 1.70651 2.47736 2.22731
H -2.10719 -3.12007 0.31518
H -3.14756 -1.28483 -0.92453
H -1.68040 -1.14145 -2.00175
H -1.56330 2.14682 0.19143
H -3.04640 1.23956 0.01967
H -1.55424 -1.47829 1.99978
H -2.97159 -0.53796 1.57858
H -1.88903 1.53698 2.55095
H -2.57707 0.93186 -2.46091
H -0.54970 1.08789 4.51492
H -0.38336 -0.69339 4.03316
H -1.85241 3.02129 -3.42793
H -1.25808 3.61865 -1.77754
45
bora-aza-Cope_TS-trans-6-conf22 E=-743.016316934 G=-742.700487 Imag-freq=1

```
C     -0.90526    -2.74959    -1.25217
C      0.11359    -1.85484    -0.67255
N     -0.16559    -0.54315    -0.40174
C     -1.62211    -0.35756    -0.07524
C     -2.47767    -0.86768    -1.24826
C     -2.10989    -2.27856    -1.59963
C      0.48427    -2.69498     1.17905
C     -2.02750     1.06248     0.35864
C     -3.50872     1.21309     0.60798
C     -4.06002     1.35486     1.81888
C      1.45814    -1.79361     1.61964
C      1.19825    -0.42469     1.85824
B      1.03725     0.28171     0.09666
C      0.94212     1.90495     0.32974
C      2.42553    -0.07752    -0.74365
C      3.65814     0.68164    -0.34377
C      0.85155     2.73138    -0.92464
C      4.75256     0.15801     0.22912
C      0.00999     3.75074    -1.15271
H     -0.59658    -3.76820    -1.46697
H      1.10186    -2.04082    -1.06748
H     -1.84062    -1.01881     0.77929
H     -2.37459    -0.20644    -2.12336
H     -3.53172    -0.83143    -0.95694
H     -2.82348    -2.89916    -2.13583
H      0.77683    -3.71929     0.96182
H     -0.53929    -2.58062     1.52832
H     -1.71539     1.77761    -0.40928
H     -1.50554     1.31409     1.28231
H     -4.15967     1.23110    -0.26536
H     -5.13232     1.47707     1.94472
H     -3.45562     1.35652     2.72403
H      2.49980    -2.09321     1.50791
H      2.01906     0.15790     2.27572
H      0.23058    -0.17330     2.29343
H      1.89938     2.15246     0.81305
H      0.17945     2.23508     1.03818
H      2.20829     0.14818    -1.80145
H      2.68459    -1.14037    -0.71022
H      3.65993     1.75500    -0.53792
H      1.55032     2.47251    -1.72232
H      5.60463     0.77591     0.50059
H      4.83054    -0.90628     0.44541
H      0.01871     4.29499    -2.09375
H     -0.71411     4.07437    -0.40712
45
bora-aza-Cope_TS-trans-6-conf23 E=-743.022183962 G=-742.706637 Imag-freq=1
C      2.40203    -1.53196     0.96117
C      0.96587    -1.25556     0.76283
N      0.55124    -0.23720    -0.04946
C      1.55372     0.37144    -0.97142
C      2.79360    -0.51610    -1.22288
C      3.29413    -1.18306     0.02656
C      0.39139    -2.99222    -0.19388
C      1.94071     1.80551    -0.51000
C      2.71268     1.93105     0.77598
C      2.28477     2.58824     1.86028
C     -0.93591    -2.65827    -0.49128
C     -1.28489    -1.62412    -1.37499
B     -0.94285    -0.04533    -0.26565
C     -1.43749     1.17406    -1.24944
C     -1.85994    -0.17873     1.08795
C     -3.33522    -0.31829     0.85152
C     -1.73174     2.48656    -0.57024
C     -4.11116    -1.32727     1.27496
C     -2.89796     3.14694    -0.60410
H      2.68341    -2.05993     1.86748
H      0.34801    -1.42132     1.63481
H      1.06280     0.49644    -1.93864
H      3.57314     0.09763    -1.68633
H      2.54490    -1.28872    -1.96548
H      4.35335    -1.39729     0.13966
H      0.58615    -3.77248     0.53787
H      1.13714    -2.91417    -0.97928
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H      1.03140     2.40674    -0.44211
H      2.53952     2.23376    -1.32696
H      3.69915     1.47004     0.80126
H      2.89563     2.66626     2.75568
H      1.30997     3.07092     1.88813
H     -1.70990    -3.01466     0.18793
H     -2.34278    -1.49504    -1.59462
H     -0.62942    -1.43238    -2.22480
H     -2.35318     0.85308    -1.76263
H     -0.70742     1.35428    -2.05073
H     -1.68968     0.76036     1.64191
H     -1.54448    -0.98814     1.75566
H     -3.80616     0.47847     0.27492
H     -0.92251     2.93420     0.00851
H     -5.17399    -1.36245     1.04892
H     -3.70780    -2.15143     1.86138
H     -3.03436     4.08957    -0.08007
H     -3.75489     2.76406    -1.15606
45
bora-aza-Cope_TS-trans-6-conf24 E=-743.012352720 G=-742.698229 Imag-freq=1
C     -1.32754    -2.74164    -0.75576
C     -0.23159    -1.83676    -0.36181
N     -0.41707    -0.48539    -0.26582
C     -1.83652    -0.14470     0.08647
C     -2.79068    -0.78454    -0.93863
C     -2.52755    -2.25168    -1.09167
C      0.18477    -2.44650     1.55937
C     -2.15242     1.35294     0.24300
C     -3.58686     1.60368     0.63399
C     -4.41530     2.45554     0.02073
C      1.32400    -1.65680     1.72717
C      1.29036    -0.24221     1.74908
B      0.89471     0.30132    -0.02263
C      0.85137     1.94647     0.10254
C      2.06412    -0.13253    -1.13224
C      3.20514    -1.03569    -0.76377
C      2.18715     2.61250     0.27871
C      4.48216    -0.66727    -0.57815
C      2.73612     3.52076    -0.54047
H     -1.08626    -3.79692    -0.83880
H      0.72543    -2.13271    -0.77193
H     -2.04887    -0.61982     1.05916
H     -2.70561    -0.27316    -1.91103
H     -3.81936    -0.62204    -0.60227
H     -3.30777    -2.89698    -1.48758
H      0.29765    -3.52609     1.49910
H     -0.76496    -2.11162     1.96974
H     -1.91635     1.89530    -0.67837
H     -1.52860     1.76510     1.03818
H     -3.94238     1.06340     1.51344
H     -5.42732     2.62046     0.37997
H     -4.10725     3.01764    -0.85856
H      2.28746    -2.13542     1.56236
H      2.23922     0.24862     1.96357
H      0.45103     0.21117     2.27782
H      0.24340     2.25467     0.96073
H      0.37168     2.36849    -0.79195
H      2.49718     0.80244    -1.50527
H      1.53871    -0.58160    -1.98944
H      2.97268    -2.09599    -0.64213
H      2.74965     2.33497     1.17241
H      5.24912    -1.38807    -0.30641
H      4.79763     0.36846    -0.68900
H      3.70695     3.96364    -0.33240
H      2.23240     3.84756    -1.44882
45
bora-aza-Cope_TS-trans-6-conf25 E=-743.018564242 G=-742.703464 Imag-freq=1
C     -1.44615    -2.63522    -0.51937
C     -0.28458    -1.86458    -0.03841
N     -0.28116    -0.49653    -0.04568
C     -1.67152     0.05863     0.07812
C     -2.55940    -0.51669    -1.03924
C     -2.50378    -2.01407    -1.05700
C     -0.18961    -2.38194     1.95640
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C     -1.78728     1.59201     0.12001
C     -3.20826     2.05773     0.31342
C     -3.83038     2.96841    -0.44271
C      0.96346    -1.66281     2.28326
C      1.02725    -0.25116     2.24696
B      1.05969     0.13237     0.38123
C      1.25815     1.76821     0.30124
C      2.37190    -0.63573    -0.26465
C      2.47234    -0.46722    -1.75194
C      2.65994     2.25564     0.54373
C      2.50791    -1.45062    -2.66450
C      3.40195     2.99049    -0.29677
H     -1.35773    -3.71719    -0.49758
H      0.65902    -2.32012    -0.30205
H     -2.07841    -0.31731     1.03225
H     -2.25872    -0.10539    -2.01632
H     -3.58784    -0.18118    -0.87384
H     -3.31297    -2.57582    -1.51693
H     -0.14903    -3.46829     1.95422
H     -1.16262    -1.96450     2.20526
H     -1.37030     2.03654    -0.78931
H     -1.20938     1.96731     0.96687
H     -3.73798     1.63021     1.16682
H     -4.84479     3.29016    -0.22386
H     -3.34436     3.42346    -1.30336
H      1.90596    -2.21001     2.29278
H      1.94938     0.20082     2.61164
H      0.13502     0.28911     2.56524
H      0.62922     2.26806     1.04744
H      0.92839     2.14107    -0.67780
H      2.45568    -1.70014    -0.01730
H      3.24900    -0.16079     0.19779
H      2.50007     0.56241    -2.11314
H      3.09825     1.99624     1.51009
H      2.55825    -1.23903    -3.72973
H      2.48893    -2.50014    -2.37465
H      4.40713     3.31334    -0.03738
H      3.02783     3.28859    -1.27489
45
bora-aza-Cope_TS-trans-6-conf26 E=-743.014877729 G=-742.699300 Imag-freq=1
C     -0.89794     2.64912     1.29449
C      0.13207     1.77903     0.69831
N     -0.16395     0.51025     0.28709
C     -1.60183     0.40095    -0.13629
C     -2.50953     0.81961     1.03228
C     -2.13303     2.18431     1.52836
C      0.64327     2.77131    -1.06008
C     -2.03482    -0.94871    -0.73145
C     -3.47952    -0.95079    -1.16243
C     -4.38244    -1.87721    -0.82334
C      1.62286     1.88221    -1.51022
C      1.35061     0.54596    -1.88094
B      1.04119    -0.31529    -0.19147
C      0.90373    -1.89041    -0.59526
C      2.37958    -0.07015     0.76123
C      3.56990    -0.92897     0.45064
C      0.63348    -2.90937     0.48900
C      4.75141    -0.50056    -0.01966
C      0.23377    -2.68551     1.74813
H     -0.57864     3.63518     1.61822
H      1.10194     1.89774     1.16001
H     -1.75005     1.15354    -0.92883
H     -2.46086     0.07908     1.84630
H     -3.54763     0.82132     0.68556
H     -2.86204     2.77616     2.07627
H      0.94268     3.76512    -0.73659
H     -0.35989     2.71235    -1.47593
H     -1.85063    -1.76260    -0.02466
H     -1.43444    -1.14032    -1.62449
H     -3.78018    -0.14309    -1.83260
H     -5.40060    -1.84244    -1.20107
H     -4.13155    -2.70195    -0.15940
H      2.66074     2.14349    -1.30564
H      2.18465    -0.02506    -2.28802
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H      0.40934     0.35649    -2.39749
H      1.86891    -2.16670    -1.04643
H      0.19528    -2.08491    -1.40930
H      2.06290    -0.28888     1.79387
H      2.72187     0.97008     0.75972
H      3.45283    -1.99925     0.62607
H      0.77838    -3.95103     0.18937
H      5.56531    -1.18982    -0.23012
H      4.94173     0.55461    -0.20988
H      0.06246    -3.50738     2.43912
H      0.05969    -1.68185     2.12699
45
bora-aza-Cope_TS-trans-6-conf27 E=-743.025529710 G=-742.711673 Imag-freq=1
C      2.39303    -1.25859     0.93451
C      0.92362    -1.14476     0.85315
N      0.33789    -0.33341    -0.07779
C      1.17838     0.19056    -1.19253
C      2.47828    -0.61027    -1.42189
C      3.15240    -0.99956    -0.13719
C      0.42967    -3.06162     0.30449
C      1.45412     1.70941    -1.01154
C      2.32613     2.11026     0.14654
C      3.41736     2.87872     0.04804
C     -0.95319    -2.89809     0.15031
C     -1.51768    -2.08394    -0.84615
B     -1.17687    -0.28593    -0.14045
C     -1.82605     0.70085    -1.27964
C     -1.94536    -0.20721     1.30585
C     -1.80941     1.13518     1.96326
C     -3.32218     0.64899    -1.40878
C     -1.23476     1.38344     3.15028
C     -4.17015     1.66575    -1.19787
H      2.81264    -1.59120     1.87925
H      0.40904    -1.18226     1.80448
H      0.58701     0.10215    -2.10648
H      3.14647    -0.01620    -2.05404
H      2.25132    -1.51979    -1.99778
H      4.23432    -1.09268    -0.10267
H      0.79805    -3.67430     1.12364
H      1.05553    -3.07127    -0.58310
H      0.48430     2.20858    -0.90284
H      1.89396     2.07916    -1.94643
H      2.00715     1.77048     1.13107
H      3.99207     3.16570     0.92450
H      3.77190     3.24562    -0.91339
H     -1.58812    -3.18107     0.98960
H     -2.60236    -2.08994    -0.93434
H     -0.99915    -2.02256    -1.80292
H     -1.40009     0.46766    -2.26685
H     -1.54222     1.74057    -1.06552
H     -1.63367    -0.98501     2.01257
H     -3.01064    -0.39194     1.10250
H     -2.20284     1.98466     1.40195
H     -3.74894    -0.30962    -1.70956
H     -1.15572     2.39291     3.54602
H     -0.82540     0.58289     3.76453
H     -5.24444     1.54449    -1.31113
H     -3.81626     2.65180    -0.90141
45
bora-aza-Cope_TS-trans-6-conf28 E=-743.027413170 G=-742.713802 Imag-freq=1
C      2.35196    -1.71354     0.90849
C      0.91016    -1.57770     0.61887
N      0.42714    -0.44087     0.03554
C      1.40967     0.54892    -0.48618
C      2.74934    -0.10140    -0.88250
C      3.25179    -1.01934     0.19825
C      0.65968    -3.06318    -0.79134
C      1.58102     1.67545     0.57399
C      2.35371     2.87125     0.08333
C      1.83319     4.09060    -0.09959
C     -0.68405    -2.83301    -1.11439
C     -1.12609    -1.66185    -1.75236
B     -1.04663    -0.34891    -0.28859
C     -1.53526     1.04631    -0.99947
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C     -2.06602    -0.89930     0.87139
C     -2.14898     0.02769     2.04874
C     -2.99509     1.11592    -1.34720
C     -1.79807    -0.25975     3.31175
C     -3.88078     2.00544    -0.87659
H      2.63933    -2.42487     1.67704
H      0.24902    -2.03544     1.34315
H      0.98170     0.99881    -1.38317
H      3.47933     0.67839    -1.11590
H      2.61477    -0.67116    -1.81406
H      4.31879    -1.12394     0.37399
H      0.92394    -3.97464    -0.26080
H      1.42945    -2.68998    -1.46023
H      2.07999     1.24467     1.45183
H      0.58547     1.99406     0.89624
H      3.41245     2.72234    -0.12917
H      2.43902     4.92018    -0.45383
H      0.78485     4.29953     0.10442
H     -1.43178    -3.44502    -0.61038
H     -2.17643    -1.61444    -2.03420
H     -0.45555    -1.19334    -2.47193
H     -0.96630     1.20762    -1.92745
H     -1.29615     1.89787    -0.34697
H     -1.82238    -1.90786     1.22515
H     -3.06137    -0.97086     0.40849
H     -2.51167     1.03538     1.83813
H     -3.35795     0.36827    -2.05534
H     -1.86526     0.48052     4.10512
H     -1.43263    -1.24646     3.59198
H     -4.92497     1.98418    -1.17809
H     -3.58951     2.78178    -0.17098
45
bora-aza-Cope_TS-trans-6-conf29 E=-743.015424468 G=-742.699956 Imag-freq=1
C     -0.47094    -2.71366    -1.30381
C      0.33963    -1.87342    -0.40543
N      0.02000    -0.56537    -0.17599
C     -1.46070    -0.33743    -0.30265
C     -1.92889    -0.78031    -1.69963
C     -1.50301    -2.19116    -1.97982
C      0.09004    -2.79631     1.45117
C     -1.93576     1.08353     0.04499
C     -3.42033     1.28045    -0.14283
C     -4.29732     1.41549     0.85873
C      0.92571    -1.95581     2.18963
C      0.66151    -0.58210     2.39327
B      1.03732     0.20509     0.68100
C      0.91123     1.81327     1.01110
C      2.61188    -0.16585     0.31660
C      3.04631     0.09021    -1.10102
C      1.10420     2.77742    -0.12889
C      4.07030     0.86138    -1.49494
C      0.34394     3.84876    -0.40132
H     -0.13356    -3.73411    -1.45733
H      1.39734    -2.08528    -0.46771
H     -1.94531    -1.01614     0.41785
H     -1.54827    -0.09613    -2.47471
H     -3.02041    -0.71678    -1.74170
H     -2.03251    -2.76954    -2.73271
H      0.39163    -3.82731     1.28466
H     -0.98490    -2.63427     1.47482
H     -1.39284     1.80724    -0.57100
H     -1.69772     1.29251     1.08824
H     -3.78738     1.33851    -1.16693
H     -5.35598     1.57174     0.67043
H     -3.98360     1.37762     1.90023
H      1.94019    -2.30650     2.37827
H      1.34230    -0.04949     3.05708
H     -0.38106    -0.29636     2.53541
H      1.75156     1.97833     1.70458
H      0.01931     2.09729     1.57818
H      2.83495    -1.21814     0.54056
H      3.25933     0.40845     0.99343
H      2.46784    -0.41296    -1.87905
H      1.95861     2.58186    -0.77550
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H      4.31630     0.98955    -2.54612
H      4.69029     1.39634    -0.77726
H      0.56454     4.50299    -1.24133
H     -0.52411     4.10595     0.20360
45
bora-aza-Cope_TS-trans-6-conf2 E=-743.018564245 G=-742.703465 Imag-freq=1
C     -1.44622    -2.63510    -0.51952
C     -0.28462    -1.86457    -0.03846
N     -0.28112    -0.49650    -0.04573
C     -1.67146     0.05870     0.07819
C     -2.55944    -0.51649    -1.03917
C     -2.50382    -2.01386    -1.05710
C     -0.18983    -2.38194     1.95638
C     -1.78713     1.59208     0.12026
C     -3.20809     2.05790     0.31356
C     -3.83021     2.96837    -0.44282
C      0.96331    -1.66295     2.28326
C      1.02730    -0.25129     2.24695
B      1.05971     0.13235     0.38131
C      1.25823     1.76819     0.30119
C      2.37191    -0.63578    -0.26460
C      2.47227    -0.46736    -1.75189
C      2.66003     2.25561     0.54363
C      2.50759    -1.45080    -2.66442
C      3.40206     2.99038    -0.29691
H     -1.35781    -3.71708    -0.49791
H      0.65896    -2.32019    -0.30201
H     -2.07831    -0.31731     1.03231
H     -2.25890    -0.10507    -2.01623
H     -3.58787    -0.18102    -0.87358
H     -3.31297    -2.57554    -1.51718
H     -0.14938    -3.46829     1.95425
H     -1.16281    -1.96438     2.20517
H     -1.37000     2.03671    -0.78895
H     -1.20930     1.96721     0.96725
H     -3.73780     1.63064     1.16711
H     -4.84461     3.29020    -0.22405
H     -3.34419     3.42318    -1.30359
H      1.90574    -2.21027     2.29281
H      1.94949     0.20059     2.61159
H      0.13515     0.28913     2.56519
H      0.62930     2.26814     1.04732
H      0.92849     2.14095    -0.67790
H      2.45575    -1.70016    -0.01716
H      3.24902    -0.16076     0.19776
H      2.50016     0.56226    -2.11314
H      3.09834     1.99626     1.51002
H      2.55788    -1.23925    -3.72966
H      2.48845    -2.50030    -2.37453
H      4.40725     3.31322    -0.03754
H      3.02795     3.28842    -1.27505
45
bora-aza-Cope_TS-trans-6-conf3 E=-743.016495881 G=-742.700669 Imag-freq=1
C      0.84098    -2.63148    -0.96728
C      1.19232    -1.40261    -0.23302
N      0.27078    -0.41726    -0.01676
C     -1.12155    -0.97214     0.04932
C     -1.42739    -1.74341    -1.24575
C     -0.37457    -2.77763    -1.51181
C      1.64292    -2.11771     1.66590
C     -2.22780     0.04512     0.36488
C     -3.59105    -0.59212     0.45417
C     -4.68044    -0.17726    -0.20123
C      2.04424    -0.89850     2.21436
C      1.16678     0.19303     2.40475
B      0.84682     0.85098     0.62839
C     -0.04532     2.20042     0.94621
C      2.31461     1.29458    -0.01441
C      2.36897     1.38573    -1.51496
C     -0.41665     3.08411    -0.21261
C      3.24145     0.75423    -2.31496
C     -1.63957     3.55000    -0.50721
H      1.63553    -3.35572    -1.11903
H      2.19195    -1.05215    -0.44460
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H     -1.12691    -1.71417     0.86531
H     -1.51503    -1.04882    -2.09664
H     -2.40629    -2.22211    -1.14377
H     -0.60543    -3.62547    -2.15195
H      2.38816    -2.89017     1.49402
H      0.63961    -2.48832     1.86238
H     -2.23359     0.84925    -0.37618
H     -2.01833     0.49535     1.33819
H     -3.67952    -1.43613     1.14099
H     -5.64425    -0.65926    -0.06226
H     -4.64395     0.65923    -0.89605
H      3.11448    -0.69329     2.23347
H      1.58074     1.06255     2.91483
H      0.15063    -0.04217     2.72326
H      0.63794     2.78987     1.57812
H     -0.92864     2.03029     1.56756
H      3.14900     0.66635     0.32026
H      2.52617     2.29388     0.39681
H      1.61680     2.01422    -1.99318
H      0.40485     3.39640    -0.85810
H      3.20543     0.86245    -3.39606
H      4.02194     0.10937    -1.91349
H     -1.80863     4.19918    -1.36266
H     -2.50991     3.29923     0.09605
45
bora-aza-Cope_TS-trans-6-conf4 E=-743.016088650 G=-742.702537 Imag-freq=1
C     -1.44822    -2.45800    -1.40184
C     -0.28276    -1.83825    -0.74407
N     -0.30856    -0.53215    -0.33952
C     -1.71131    -0.12036     0.01830
C     -2.62397    -0.31695    -1.20308
C     -2.53392    -1.73009    -1.69779
C     -0.08945    -2.91254     1.02180
C     -1.89632     1.27352     0.64025
C     -3.32141     1.51779     1.06989
C     -4.04953     2.59163     0.74657
C      1.00849    -2.23583     1.56196
C      0.97159    -0.87274     1.93665
B      1.01634     0.00145     0.23754
C      1.20178     1.59597     0.57670
C      2.35007    -0.52282    -0.58906
C      3.67019    -0.28234     0.08833
C      1.12788     2.49684    -0.62767
C      4.70044     0.43058    -0.38806
C      2.09696     3.30831    -1.07552
H     -1.33866    -3.49085    -1.71843
H      0.65600    -2.17205    -1.16138
H     -2.05534    -0.83978     0.77993
H     -2.36333     0.39660    -2.00093
H     -3.65381    -0.08648    -0.91280
H     -3.34442    -2.14455    -2.29207
H      0.03487    -3.94381     0.70096
H     -1.08810    -2.66455     1.37394
H     -1.58023     2.06143    -0.04882
H     -1.27427     1.34387     1.53572
H     -3.75854     0.76141     1.72436
H     -5.05997     2.72575     1.12261
H     -3.65789     3.37265     0.09806
H      1.98848    -2.69554     1.43352
H      1.85356    -0.47814     2.44011
H      0.04040    -0.50424     2.36714
H      2.19647     1.70789     1.02628
H      0.49744     1.95709     1.33281
H      2.35868    -0.02538    -1.57053
H      2.31627    -1.59996    -0.79621
H      3.79924    -0.75944     1.06265
H      0.19515     2.47393    -1.19416
H      5.62539     0.53868     0.17316
H      4.64867     0.93463    -1.35106
H      1.95975     3.92151    -1.96294
H      3.05944     3.37881    -0.57310
45
bora-aza-Cope_TS-trans-6-conf5 E=-743.015853762 G=-742.701003 Imag-freq=1
C     -1.78268    -2.53213    -0.54790
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C     -0.58136    -1.87139    -0.00860
N     -0.38286    -0.52476    -0.13449
C     -1.68719     0.22096    -0.22195
C     -2.53637    -0.35140    -1.37213
C     -2.68314    -1.83803    -1.25471
C     -0.76464    -2.19703     2.03067
C     -1.56922     1.75424    -0.33250
C     -2.90069     2.44821    -0.49549
C     -3.49661     3.16757     0.46230
C      0.45460    -1.62836     2.40441
C      0.74193    -0.25211     2.25508
B      0.99331    -0.03738     0.37688
C      1.42549     1.54310     0.21636
C      2.22891    -1.02529    -0.10024
C      2.36097    -1.13079    -1.59427
C      2.81663     1.87916     0.68136
C      3.41168    -0.75142    -2.33678
C      3.76482     2.50364    -0.03079
H     -1.84736    -3.60848    -0.42160
H      0.30892    -2.47484    -0.11212
H     -2.23655     0.01306     0.71083
H     -2.10080    -0.08049    -2.34731
H     -3.52629     0.11326    -1.33853
H     -3.51171    -2.33411    -1.75376
H     -0.89669    -3.27205     2.12261
H     -1.67730    -1.61464     2.13346
H     -0.92557     2.00730    -1.18277
H     -1.09981     2.14513     0.56925
H     -3.38652     2.37043    -1.46723
H     -4.44947     3.66129     0.29247
H     -3.04897     3.28837     1.44694
H      1.29478    -2.30647     2.55422
H      1.68710     0.08850     2.67633
H     -0.07919     0.44115     2.44116
H      0.75338     2.18685     0.79467
H      1.32804     1.85825    -0.83156
H      2.13433    -2.04013     0.30983
H      3.16555    -0.63360     0.31433
H      1.50034    -1.55114    -2.11958
H      3.05769     1.61116     1.71231
H      3.41048    -0.85501    -3.41922
H      4.30226    -0.31892    -1.88556
H      4.74064     2.72846     0.39276
H      3.59751     2.80328    -1.06390
45
bora-aza-Cope_TS-trans-6-conf6 E=-743.016295220 G=-742.700296 Imag-freq=1
C     -1.26284    -2.60471    -1.33034
C     -0.15386    -1.90986    -0.65113
N     -0.22226    -0.57404    -0.36630
C     -1.64608    -0.14112    -0.14763
C     -2.47956    -0.47628    -1.39675
C     -2.33553    -1.92521    -1.75667
C     -0.08384    -2.82759     1.20491
C     -1.83175     1.32078     0.29584
C     -3.27955     1.72061     0.44643
C     -3.88466     1.93865     1.61976
C      0.98329    -2.10861     1.75171
C      0.93305    -0.71848     2.00415
B      1.05726     0.02507     0.24543
C      1.23160     1.63650     0.50772
C      2.43007    -0.55674    -0.48138
C      3.73172    -0.08142     0.09891
C      1.36875     2.47438    -0.73366
C      4.69905     0.58674    -0.54548
C      0.73009     3.62350    -1.00108
H     -1.11956    -3.65878    -1.54790
H      0.81600    -2.26162    -0.97203
H     -2.04314    -0.76746     0.66791
H     -2.19214     0.16804    -2.24282
H     -3.53127    -0.25897    -1.18726
H     -3.10061    -2.40409    -2.36259
H      0.05258    -3.88313     0.98333
H     -1.10078    -2.54769     1.46978
H     -1.34672     1.98218    -0.42913
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H     -1.34215     1.46465     1.25942
H     -3.85329     1.86127    -0.46891
H     -4.92679     2.24124     1.67461
H     -3.35552     1.82463     2.56399
H      1.96612    -2.57902     1.72408
H      1.79061    -0.28549     2.51854
H     -0.01712    -0.31295     2.35243
H      2.19337     1.70144     1.03919
H      0.50101     2.09207     1.18022
H      2.39788    -0.29055    -1.54931
H      2.47152    -1.65277    -0.44873
H      3.90041    -0.32372     1.15095
H      2.07293     2.10463    -1.48023
H      5.61615     0.88649    -0.04453
H      4.60171     0.85944    -1.59501
H      0.89955     4.16508    -1.92845
H      0.01915     4.06120    -0.30246
45
bora-aza-Cope_TS-trans-6-conf7 E=-743.018564235 G=-742.703465 Imag-freq=1
C     -1.44637    -2.63506    -0.51955
C     -0.28471    -1.86458    -0.03852
N     -0.28116    -0.49651    -0.04574
C     -1.67144     0.05879     0.07838
C     -2.55971    -0.51640    -1.03877
C     -2.50406    -2.01376    -1.05687
C     -0.18982    -2.38211     1.95613
C     -1.78696     1.59219     0.12024
C     -3.20786     2.05819     0.31356
C     -3.82986     2.96877    -0.44279
C      0.96337    -1.66319     2.28307
C      1.02741    -0.25155     2.24685
B      1.05975     0.13222     0.38131
C      1.25838     1.76805     0.30138
C      2.37186    -0.63592    -0.26478
C      2.47213    -0.46728    -1.75206
C      2.66022     2.25537     0.54378
C      2.50713    -1.45059    -2.66475
C      3.40220     2.99026    -0.29671
H     -1.35795    -3.71705    -0.49810
H      0.65882    -2.32020    -0.30223
H     -2.07815    -0.31706     1.03262
H     -2.25947    -0.10489    -2.01589
H     -3.58810    -0.18097    -0.87288
H     -3.31329    -2.57540    -1.51689
H     -0.14939    -3.46847     1.95388
H     -1.16277    -1.96457     2.20507
H     -1.36985     2.03663    -0.78907
H     -1.20904     1.96740     0.96713
H     -3.73762     1.63101     1.16711
H     -4.84421     3.29074    -0.22400
H     -3.34380     3.42351    -1.30357
H      1.90577    -2.21055     2.29254
H      1.94964     0.20025     2.61151
H      0.13530     0.28888     2.56519
H      0.62954     2.26794     1.04763
H      0.92858     2.14096    -0.67763
H      2.45562    -1.70035    -0.01751
H      3.24903    -0.16104     0.19759
H      2.50021     0.56239    -2.11315
H      3.09861     1.99584     1.51008
H      2.55737    -1.23888    -3.72996
H      2.48780    -2.50013    -2.37503
H      4.40742     3.31303    -0.03738
H      3.02800     3.28849    -1.27476
45
bora-aza-Cope_TS-trans-6-conf8 E=-743.017123896 G=-742.701087 Imag-freq=1
C     -0.72403    -2.80222    -1.22711
C      0.25551    -1.84402    -0.68038
N     -0.11593    -0.57470    -0.32912
C     -1.55369    -0.53948     0.10533
C     -2.44228    -1.06507    -1.03427
C     -1.98629    -2.42502    -1.47183
C      0.83983    -2.71542     1.10043
C     -2.06721     0.80482     0.64226
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C     -3.49924     0.72854     1.10785
C     -4.47447     1.56664     0.74044
C      1.76100    -1.74603     1.50922
C      1.40053    -0.41675     1.82787
B      1.04093     0.33888     0.11566
C      0.81322     1.93585     0.42455
C      2.38794     0.14358    -0.83762
C      3.57468     0.99618    -0.49121
C      0.55168     2.79207    -0.78501
C      4.75276     0.55258    -0.02697
C     -0.39864     3.73009    -0.91178
H     -0.34637    -3.78080    -1.50791
H      1.22324    -1.92423    -1.15412
H     -1.64781    -1.26382     0.93195
H     -2.44290    -0.36012    -1.88097
H     -3.47625    -1.11335    -0.67864
H     -2.68053    -3.08461    -1.98656
H      1.20464    -3.69971     0.81738
H     -0.15994    -2.70893     1.52849
H     -1.95627     1.59031    -0.10999
H     -1.46242     1.08608     1.50815
H     -3.72611    -0.05927     1.82880
H     -5.47934     1.47992     1.14449
H     -4.29877     2.36801     0.02573
H      2.81338    -1.94436     1.30827
H      2.19660     0.22243     2.20888
H      0.45107    -0.27140     2.34396
H      1.77608     2.25782     0.84932
H      0.07764     2.16692     1.19814
H      2.07212     0.39150    -1.86519
H      2.74196    -0.89142    -0.87345
H      3.46492     2.07243    -0.63070
H      1.21209     2.63132    -1.63915
H      5.56437     1.23494     0.21221
H      4.94268    -0.50820     0.12876
H     -0.51093     4.30481    -1.82772
H     -1.09427     3.95416    -0.10518
45
bora-aza-Cope_TS-trans-6-conf9 E=-743.015853750 G=-742.701001 Imag-freq=1
C     -1.78277    -2.53216    -0.54781
C     -0.58143    -1.87144    -0.00855
N     -0.38290    -0.52482    -0.13447
C     -1.68722     0.22093    -0.22195
C     -2.53637    -0.35143    -1.37214
C     -2.68322    -1.83805    -1.25464
C     -0.76463    -2.19696     2.03073
C     -1.56920     1.75421    -0.33247
C     -2.90063     2.44827    -0.49536
C     -3.49618     3.16810     0.46230
C      0.45460    -1.62825     2.40447
C      0.74199    -0.25205     2.25508
B      0.99325    -0.03748     0.37679
C      1.42554     1.54295     0.21620
C      2.22883    -1.02544    -0.10027
C      2.36087    -1.13097    -1.59430
C      2.81669     1.87892     0.68126
C      3.41144    -0.75129    -2.33685
C      3.76483     2.50364    -0.03075
H     -1.84751    -3.60850    -0.42145
H      0.30884    -2.47492    -0.11210
H     -2.23659     0.01304     0.71082
H     -2.10072    -0.08060    -2.34731
H     -3.52627     0.11328    -1.33864
H     -3.51185    -2.33411    -1.75361
H     -0.89667    -3.27198     2.12273
H     -1.67729    -1.61457     2.13351
H     -0.92558     2.00727    -1.18277
H     -1.09972     2.14505     0.56926
H     -3.38674     2.37016    -1.46694
H     -4.44901     3.66190     0.29253
H     -3.04825     3.28922     1.44677
H      1.29477    -2.30637     2.55436
H      1.68719     0.08854     2.67627
H     -0.07907     0.44129     2.44109
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H	0.75346	2.18685	0.79437
H	1.32821	1.85799	-0.83177
H	2.13427	-2.04026	0.30984
H	3.16547	-0.63371	0.31425
H	1.50034	-1.55159	-2.11958
H	3.05780	1.61062	1.71212
H	3.41024	-0.85487	-3.41928
H	4.30189	-0.31849	-1.88564
H	4.74065	2.72838	0.39284
H	3.59748	2.80354	-1.06378

References

[S1] L. I. Zakharkin and V. I. Stanko, *Bull. Acad. Sci. USSR, Div. Chem. Sci*., 1960, **9**, 1774 (*Izv. Akad. Nauk SSSR, Ser. Khim*., 1960, 1896).

[S2] Yu. N. Bubnov, E. A. Shagova, S. V. Evchenko and A. V. Ignatenko, *Russ. Chem. Bull., Int. Ed*., 1994, **43**, 645 (*Izv. Akad. Nauk, Ser.Khim*., 1994, 693).

[S3] N. Yu. Kuznetsov, V. N. Khrustalev, I. A. Godovikov, and Yu. N. Bubnov, *Eur. J. Org. Chem*., 2006, 113. 1994.

[S4] N. Yu. Kuznetsov, K. A. Lyssenko, A. S. Peregudov and Yu. N. Bubnov, *Russ. Chem. Bull*., 2007, **56**, 1569 (*Izv. Akad. Nauk, Ser.Khim*., 2007, 1510).

[S5] Yu. N. Bubnov, E. E. Demina and A. V. Ignatenko, *Russ. Chem. Bull*., 1997, **46**, 1306 (*Izv. Akad. Nauk, Ser.Khim*., 1997, 1361).

[S6] N. Yu. Kuznetsov, V. N. Khrustalev, I. A. Godovikov and Yu. N. Bubnov, *Eur. J. Org. Chem*., 2006, 113.

[S7] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision D.01*, Gaussian, Wallingford, CT, 2009.