Boltzmann Analysis of the trans- vs. cis-Menthone Equilibrium Ratio from DFT Energies

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To see the structures of the .pdb files (Protein Data Bank) in a folder that I have provided on the course website, you can use Chem3D or Avogadro v.1.99. As a Mac user, I prefer the latter because it avoids the hassles of using Chem3D via Citrix at apps.umn.edu. Avogadro is also more robust in the things it can do. Avogadro is freely downloadable (and usable) from:

https://two.avogadro.cc/install/index.html

I have also provided on the website a folder of .png files, where you can see a static image of each of the conformers resulting from the DFT optimizations.

When you attempt to download from our website the above folders as well as the Excel file at "Excel file of the DFT energies for the conformations of the trans- and cis-menthones (posted 11-13-24)," you will likely see an alert message (on my Mac it reads "Insecure downloads blocked" but I am given the option to "Keep", at which point the folder is fully functional). This is a normal function for the website because the server on which it is housed is not able to handle https secure files and folders. Until you instruct the download to "Keep" the file or folder, it may show up in your Downloads folder as "Unconfirmed#######.crdownload." At some point you may be asked ~"Do you want to open it anyway?" Answer "yes" and the file or folder will then be readable in your Downloads.

The Exercise, due by the end of lab, Tuesday, December 3rd.

Create a similar spreadsheet modeled after the templates you can view in the PDF at "Template (a 2 page PDF) for Creating Your Excel Spreadsheet for the Menthone Boltzmann Equilibrium Values (posted 11-14-24)" from the website. Use the energies of the optimized DFT structures that Jingyang calculated. They are found in "Excel file of the DFT energies for the conformations of the trans- and cis-menthones (posted 11-13-24)." *Note: The conformation #s in that file (#1-7 for the cis and #1-8 for the trans) are not ordered by their relative energies.* Compute the K_{eq} from the DFT energy values by analogy to what I have done in the template Excel sheets in the PDF file.

Turn in:

1. **A printout of the final Excel spreadsheet you created in which you have calculated:**
   a. **the Keq from the Boltzmann averaged energies of the full ensemble of conformations**
   b. **the Keq using only the two lowest energy (i.e., most stable) conformer of each isomer**

2. **A one-paragraph description/discussion in which you summarize the results of your treatment of the calculations and a comparison with the experimental K_{eq} that you measured in Experiment 2. (Include the temperature at which you carried out your equilibration.)**