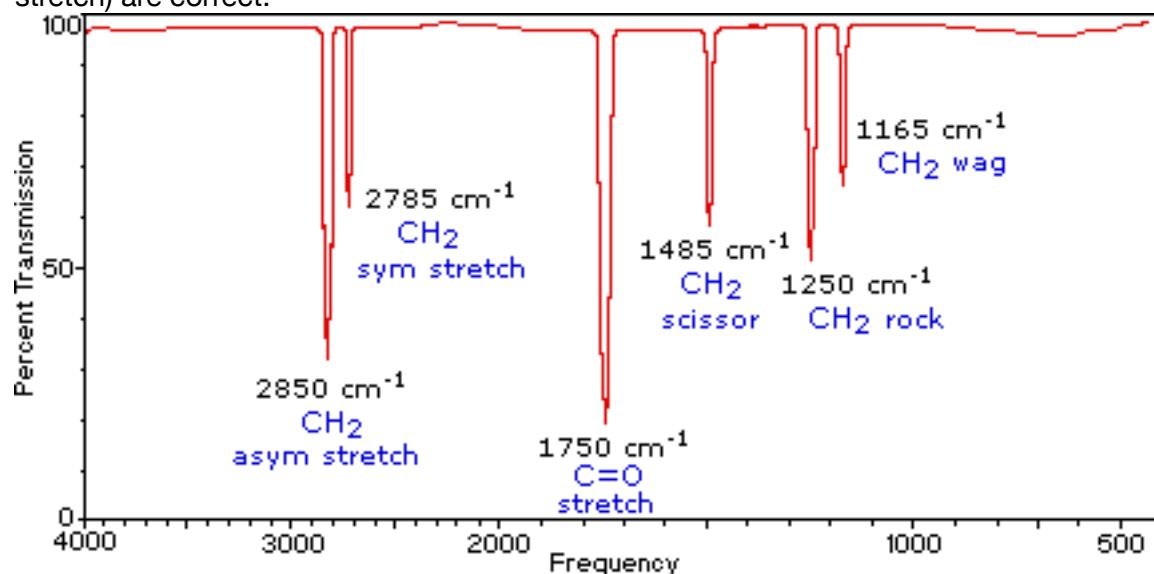
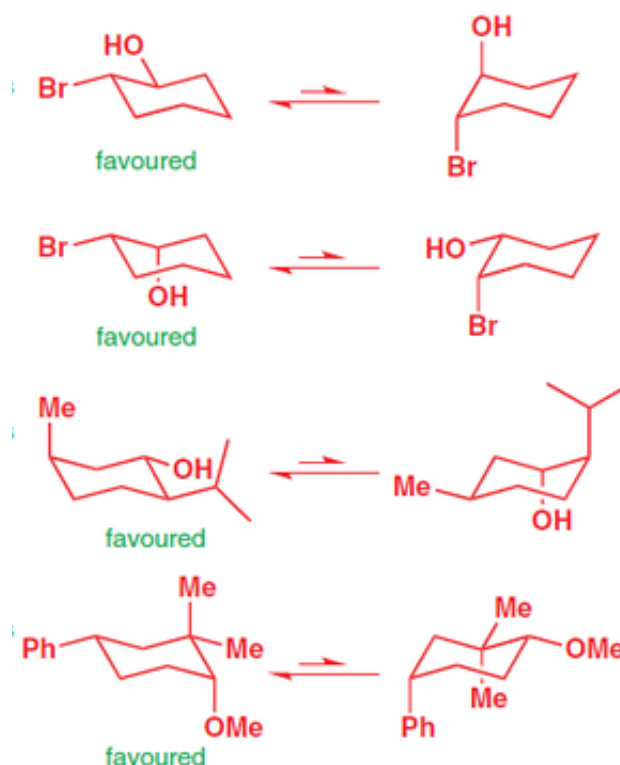


- (1) Model the Diels-Alder reaction between butadiene and ethylene to form cyclohexene. Show using IRC calculations that the transition state obtained corresponds to this reaction.
- (2) Perform conformational analysis on ethane, propane and butane. Plot all the three energy curves in the same graph. Explain the observed trend of change in energies.
- (3) Below is the Infrared (vibrational) spectrum of formaldehyde obtained using experiments. Compute the spectrum using HF/STO-3G method and compare the two. Check if the assignment of the frequencies of the peaks (for eg.  $2850\text{ cm}^{-1}$  is assigned as asymmetric stretch) are correct.



Source: [chemistry.msu.edu](http://chemistry.msu.edu)

- (4) Verify the following by calculating the energy differences between the two conformational states in each case.



Source: [qph.fs.quoracdn.net](http://qph.fs.quoracdn.net)