Computational analysis of ro-vibrations of vinyl alcohol and the formation of 2-chloroethanol

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The vibrational signatures and reaction pathways of small molecules are of interest when trying to identify a molecule in the interstellar medium, or consider the plausibility of a molecule being present at all. For example, in 2001, Turner and Apponi positively identified vinyl alcohol in the molecular cloud, Saggitarius B2(N). Researchers continue to look for signatures of vinyl alcohol in the interstellar medium since it is an important intermediate in many organic reactions and may therefore play a role in the formation of complex organic molecules in space. We used computational methods to calculate ro-vibrational constants of both syn- and anti-vinyl alcohol and compared them to experiments performed using far-infrared spectroscopy. Specifically, we calculated the anharmonic vibrations using second order vibrational perturbation theory (VPT2) at the CCSD(T)/cc-PVTZ level of theory. The vibrational frequencies, rotational constants and quartic centrifugal distortion constants are in good agreement with experiment and should be useful in identifying anti vinyl alcohol in the interstellar medium. Furthermore, several reaction pathways for the formation of 2-chloroethanol have been investigated. Intrinsic reaction coordinate (IRC) calculations were performed at the MP2/cc-PVTZ level-of-theory for both solvated and gas-phase reactions of oxirane with HCl, and ethylene glycol with HCl. The results of these calculations show that all of these reactions are exothermic with reasonable barrier heights.