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Spectroscopic and Theoretical Investigations of the Conformations and -type Hydrogen Bonding of 2-Cyclohexen-1-ol ESTHER OCOLA, JAAN LAANE, Texas AM University — Infrared and Raman spectra of 2-cyclohexen-1-ol have been collected for its liquid and vapor states. As confirmed by *ab initio* (MP2/cc-pVTZ) and density functional theory (B3LYP/cc-pVTZ) calculations, this molecule can exist as six different conformers, possibly only five, if the third most abundant conformer and the first most abundant conformer have no energy barrier between them. The conformers can interconvert by the twisting of the six-membered ring or by torsional rotation of the –OH bond. This can be shown by a potential energy surface and its topological map. The lowest energy conformers **A** and **B** have the –OH bond oriented towards the C=C bond and possess an intramolecular π-type hydrogen bonding. The calculated distance from the hydrogen atom of the –OH group to the middle of the C=C bond is 2.7 Å for **A**, whereas for **B** it is 3.0 Å. The highest energy form lies 401 cm^{-1} (1.15 kcal/mol) higher in energy. This conformer has an interatomic distance of 3.2 Å between the hydrogen atom of the –OH group and the C=C bond. The experimentally observed infrared and Raman frequencies agree very well with the calculations and clearly show the presence of these conformers.

Esther Ocola
Texas A
M University

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