AB INITIO CALCULATION OF CONFORMATIONS AND INFRARED SPECTRA OF MESO AND RACEMIC 2,4-PENTANEDIOL

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The infrared spectra of meso-2,4-pentanediol and racemic-2,4-pentanediol were measured in an argon isolated matrix at 20 K. The absorptions were obtained using a low temperature cryostat and a Fourier transform infrared spectrophotometer. The meso and racemic forms of the diol were separated by means of a spinning band distillation column. Ab initio molecular orbital calculations were performed to obtain the equilibrium geometry, vibrational frequencies, force fields, and infrared intensities. The calculations were done at the Hartree-Fock level using 6-31++G** basis set.