CCSD(T) STUDY OF THE FAR-INFRARED SPECTRUM OF ETHYL METHYL ETHER

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The molecular structure and the far infrared spectrum of ethyl methyl $ether - d_0$ are investigated using state-of-the-art CCSD(T) ab initio calculations. We provide the geometry of the two conformers (trans and gauche), the corresponding harmonic and anharmonic fundamentals, the torsional barriers and the three dimensional Potential Energy Surface depending on the vibrational motion responsible of the non-rigidity. The dependence of the spectroscopic parameters with the torsional motion is detailed.
From the Potential Energy Surface, the rotorsional energy levels are calculated variationally with a flexible model depending on the three large amplitude coordinates [a]. We provide the far infrared frequencies and intensities at room temperature and the rotational parameters computed for the lowest torsional energy levels. Results are compared with available experimental data [b] [c].

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