VIBRATIONAL SPECTRA OF A NON RIGID MOLECULE : ETHANE

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In this work the ethane molecule has been treated as a non-rigid molecule by considering the internal rotation of one of the methyl groups. The potential energy adapted to the molecular symmetry has been expressed as a function of the C-C stretching normal mode coordinate and the internal rotation angle (theta). The Far-Infrared spectra has been calculated and compared with: 1) A model in which the internal rotation is not considered and 2) experimental results obtained in the literature. Also the potential parameters are compared with the ones obtained by experimental spectra fitting.