ETHANE C-H STRETCHING VIBRATIONAL SPECTRA COUPLING

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In previous work it has been studied the ethane vibrational spectra , being considered as a non-rigid molecule. In this work we are interested in studying in particular de symmetric and anti-symmetric c-h vibrational modes. Those normal modes vibrational frequencies are quite close and we are using a Hamiltonian model in which both are coupled togheter. In this case the couple among then is stronger than the coupled with the internal rotational mode and the results are compared with the ones reported in the literature (J.M. Fernandez and S. Montero, J. Chem. Phys. 118-6, 2657,(2003)).