

ETHANE C-H STRETCHING VIBRATIONAL SPECTRA COUPLING

MARIA VILLA, *Departamento de Quimica. Universidad Autonoma Metropolitana, Av. San Rafael Atlixco 186, Col Vicentina, Iztapala, Mexico D.F. 09340, MEXICO*; MA. LUISA SENENT, *Departamento de Astrofisica Molecular e Infrarroja, Instituto de Estructura de la Materia, C.S.I.C., Serrano 113B, Madrid 28006, SPAIN*; and DAVID R. HIDALGO, *Departamento de Quimica. Universidad Autonoma Metropolitana, Av. San Rafael Atlixco 186, Col Vicentina, Iztapala, Mexico D.F. 09340*.

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 together. In this case the couple among them 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)).