ETHANE ASYMMETRIC C-H STRETCHING VIBRATIONAL SPECTRA

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 this work we continue studying the ethane vibrational spectra, being considered as a non-rigid molecule. The Θ internal rotational angle and the symmetric and anti-symmetric CH stretching normal modes will be the variables under study. Using ab-initio calculations a three dimentional potential is obtained, and finally a three dimentional Far-infrared and infrared spectra will be presented. The results obtained will be compared with the ones reported in the literature.