Equilibrium constants of the conformational interconversion and vibrational analyses of vinylfluorogermanes.   Forner, Wolfgang; Badawi, Hassan M.; Seddigi, Zaki S

Abstract

The rotational potential energy surfaces for vinylfluorogermanes, $CH_2:CHGeH_2F$ and $CH_2:CHGeHF_2$ were investigated by DFT-B3LYP/6-311++G** and ab initio MP2/6-311++G** calcns. The potential functions for the internal rotation of the GeH_nF_{3-n} rotors were calcd. and it was found that they are very similar for the two mols. Both mols. exhibit a conformational equil. between the two stable cis- and gauche-forms, where in both cases the trans conformation is one of the two transition states. In the case of the vinylmonofluorogermane the gauche form is slightly lower than the cis one, while in the case of vinyldifluorogermane the two forms are nearly degenerate. The equil. consts. of the two equil. were calcd. and are presented. The vibrational frequencies of the two mols. in their stable conformations were computed. The potential energy distributions, PED, among the symmetry coordinates of the normal modes of the vinylfluorogermanes were calcd. from normal coordinate calcns. and a complete assignment of all spectral modes is provided. Further the IR and vibrational Raman spectra of the two conformational equil. were plotted and shown in this work. It is pointed out, that in contrast to previous findings in a similar system, in the present case DFT total energies seem to be of similar reliability as MP2 ones.