

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Theoretical Comparative Study of the Structure, Dynamics and Electronic Properties of Five Allyl Molecules: Allicin, Methyl Propyl Disulfide (MPD), Allyl Methyl Sulfide (AMS), S-allyl cysteine (SAC) and S-allyl mercaptocysteine (SAMC)¹ EMINE DENIZ CALISIR , SAKIR ERKOC, Department of Physics, Middle East Technical University, 06531 Ankara, Turkey, HANDAN YILDIRIM , ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, Kansas State University, Manhattan, USA, MAHMUT SELVI, FIGEN ERKOC, Department of Biology Education, Gazi University, 06500 Ankara, Turkey — The structural, dynamics and electronic properties of five allyl molecules have been investigated theoretically by performing semi-empirical molecular orbital (AM1 and PM3), ab-initio (RHF) and density functional theory calculations. The geometry of the molecules have been optimized, the vibrational spectra and the electronic properties of the molecules have been calculated in their ground states in gas phase. For each molecule, we found that the optimized geometries resulting from calculations based on the three levels of accuracy, to be very similar. However, we found that an accurate description of the vibrational properties of these molecules necessitates calculations at the ab-initio level. The electronic structures of these molecules were performed at the DFT level, resulting in an accurate description of the HOMO-LUMO gap and the local charges.

¹Work supported in part by NSF under grant No: INT_0244191

Handan Yildirim

Date submitted: 05 Dec 2005

Electronic form version 1.4