

Interpretation of Vibrational Spectra of Allyl Acrylate

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Esters of acrylic acid are widely used as monomers for acrylic polymers, which are further used for production of dyes, paper, textiles, glues, adhesives, paints etc. Demand for acrylic acid was estimated in 2005 to increase ca. 4.2 percent a year [1]. More than half of the world production of acrylic acid is used to synthesize various acrylic acid esters: mainly methyl, ethyl, n-butyl, and 2-ethylhexyl acrylates. Since few years we are developing a technology for production of acrylates from waste glycerol, therefore, we are also involved in a deeper characterization of particular products such as allyl acrylate. Allyl acrylate is used for curing polymeric materials, such as those utilized in dentistry.

The vibrational spectra of allyl acrylate (Fig. 1) were not interpreted in details, so far. This is a laborious task because of numerous conformations that the allyl acrylate molecule can adopt (Fig. 2). Our population analysis and IR and Raman spectra calculations of the allyl acrylate conformers were performed at the B3LYP/aug-cc-pVDZ level. Based on these calculations, there are seven conformers which are less stable than the most stable one by less than 1.0 kcal/mol, only. To interpret the experimental spectra, the calculations were followed by the potential energy distribution analysis.

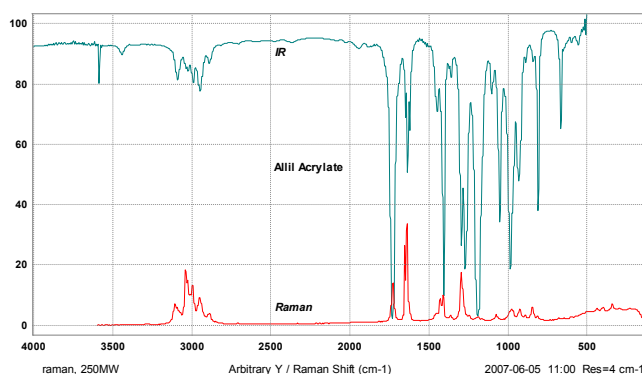


Fig. 1: The IR and Raman spectra of allyl acrylate.

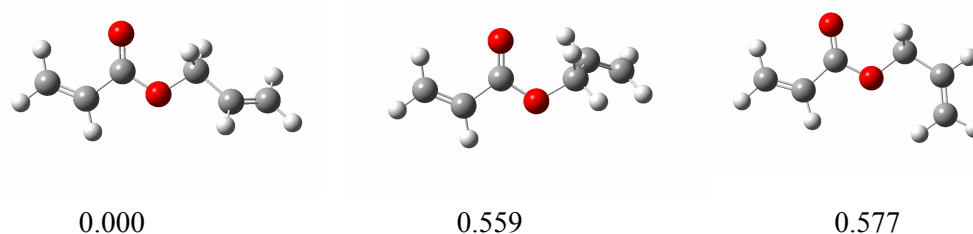


Fig. 2: The most stable three conformers of allyl acrylate calculated at the B3LYP/aug-cc-pVDZ level accompanied with the Gibbs free energy differences in kcal/mol.

[1] Acrylic Acid & Derivatives to 2005 - Market Size, Market Share, Market Leaders, Demand Forecast and Sales, © Copyright 2006 The Freedonia Group, Inc. 767 Beta Drive Cleveland, Ohio 44143.