

DFT Study of Molecular Structure and Vibrations of 3-Glycidoxypropyltrimethoxysilane

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Organofunctional alkoxy silanes have a widespread application in the polymer industries. Possessing both organic and inorganic properties, these chemicals react with organic polymers and with inorganic substrates, pigments or fillers, forming durable covalent bonds across the interface. 3-glycidoxypropyltrimethoxysilane (GPTMS) is one of the most widely applied organofunctional alkoxy silanes. It has two functional groups on the opposite sites of the molecule. Methoxy groups, at one end of the molecule, are transformed through hydrolysis into silanol groups which can interact and form a silicate network during the condensation process. On the other side, by using curing agents at room temperature, epoxy ring opening and organic network formation can be achieved.

Changes in the vibrational spectra of GPTMS during these processes are frequently used for monitoring the relevant dynamics. The knowledge and assignment of the vibrational spectra of individual GPTMS molecule may be helpful in understanding the nature of the interactions involved. Therefore, we have investigated molecular structure and vibrational frequencies of GPTMS by density functional theory (DFT) calculations using Becke's three-parameter exchange functional combined with Lee-Young-Parr correlation functional (B3-LYP) and standard basis set 6-311++G(d,p). In order to reveal all possible conformations of GPTMS, potential energy scan has been performed in three dihedral angles SiCCC, CCCO and OCCO. The calculations predict the existence of seven different conformations: 1-*ttg*, 2-*gtg*, 3-*gtg*, 4-*tgg*, 5-*tgg*, 6-*ttg* and 7-*ttt*. Mostly, they have negligible differences in their calculated vibrational spectra. The lowest energy conformer according to our calculations is 6-*ttg*. The complete assignment of the measured vibrational spectra is given for this most stable molecule using the correspondence of observed and calculated frequencies, calculated Raman activities and IR intensities, characteristic group frequencies and comparison with aminopropylsilanetriol [1] and gamma-aminopropyltriethoxysilane [2]. Comparing the results of spectroscopic measurements (Raman and IR spectra of liquid sample were recorded) and DFT calculations it was possible to distinguish four pairs of corresponding vibrational bands characteristic for three different groups of conformers. Bands at 1480 cm⁻¹, 1441 cm⁻¹ and 1313 cm⁻¹ are ascribed to 6-*ttg* and 7-*ttt* conformers. Corresponding normal modes in the remaining five conformers generate the same bands at 1466 cm⁻¹, 1414 cm⁻¹ and 1341 cm⁻¹. Strong Raman band at 612 cm⁻¹ is attributed to SiO stretching vibration in molecules 2-*gtg* and 3-*gtg*, while the similar normal mode in other five conformers gives rise to the strong Raman band at 642 cm⁻¹.

A comparison of experimental and calculated results points to the possible co-existence of all conformers in the liquid GPTMS.

[1] L. Bistričić, V. Volovšek, V. Dananić, I. Movre Šapić, *Spectrochim. Acta A* 64 (2006) 327-337

[2] L. Bistričić, V. Volovšek, V. Dananić, *J. Mol. Struct.* 834-836 (2006) 355-363