# DFT Vibrational Study of Organic-Inorganic Hybrid Polymers Based on 3-Glicidoxypropyltrimethoxysilane

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Organic-inorganic hybrid polymers have recently attracted much atention since they combine the advantages of organic polymers, like toughness and flexibility, with those of inorganic components such as high heat resistance, good optical and mechanical properties. The objective of this research is the characterization of the structure of organic-inorganic hybrid polymers based on 3-glicidoxypropyltrimethoxysilane (GPTMS). GPTMS molecule possesses both epoxy and silicon alkoxide functionality and so interlinked organic-inorganic networks can be formed. Hydrolysis of the methoxy groups gives silanol groups (SiOH) which can condense and form siloxane (SiOSi) bonds. The epoxy ring can be opened and polymerized to form organic network.

In this work polymer with inorganic SiOSi bonds (GPTMS-1) and hybrid polymer obtained from GPTMS/APTES (3-aminopropyltrietoxysilane) system (GPTMS-2) was prepared by a sol-gel process. The structure of polymers was characterized by vibrational spectroscopy (Raman and IR). The interpretation of vibrational spectra is supported by the normal coordinate analysis based on density functional theory (DFT) calculations. A comprehensive conformational and vibrational analysis of expected polymer structures has been carried out by DFT calculations using Becke's three-parameter exchange functional in combination with the Lee-Young-Parr correlation functional (B3-LYP) and standard 6-311+G(d,p) basis set.

The comparison of theoretical spectra with the experimental data enabled us to extract the characteristic vibrational bands of different polymer structures. The free GPTMS molecule has characteristic fundamentals at 1256 $cm^{-1}$ (mode of epoxy ring) as well as SiO stretching modes at 642 and at 612 $cm^{-1}$ [1]. The SiO stretching vibrations are not evident in spectra of GPTMS-1 polymer indicating the condensation of methoxy groups and possibility of inorganic SiOSi polymerization. The intense Raman band observed at 1136 $cm^{-1}$ and assigned to the SiOSi stretching vibrations suggests the ladder-type structure of GPTMS-1 polymer [2]. In vibrational spectra of GPTMS-2 polymer the absence of 1256 $cm^{-1}$ band and $NH_2$ stretching modes at ~ 3400 $cm^{-1}$ from APTES [3] resulted from reaction between primary amine and epoxy ring. The analysis of vibrational spectra has shown that the structure of GPTMS-2 polymer obtained by simultaneous inorganic and organic polymerization depends on the presence of water and solvents.

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