

Vibrational Spectroscopy as Useful Tool in Investigation of Phase Transition and Structural Research

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The infrared and Raman spectroscopy can be used very often for determination of weak and strong interaction as strength of chemical bonds and structure of molecule. On the basis of vibrational spectra analysis the functional groups in molecules can be identified and described.

More useful information about chemical interaction are obtained when vibrational spectroscopy on monocrystal sample with polarized light is used. The characteristic bands assigned to stretching vibrations of hydrogen bonds are observed on powder IR and Raman spectra very well, but only spectroscopy on monocrystals with polarized light gives full information about behavior of hydrogen bond network in investigated compounds.

The polarized vibrational spectra were successfully used for detailed analysis of hydrogen bonds network in relation to the Betaine*H₂SeO₃ crystal structure[1], hydrochloride diglycine hydrochloride[2], pentacaesium trihydrogentetraselenate monohydrate[3], monoglycine dihydrogenphosphate[4] and ferroelectric glycinium hydrogenphospite (GPI)[5].

On the other hand the advanced low temperature vibrational spectroscopy can be used together with DSC measurement for detection and determination of mechanism of structural phase transition. This method was successfully used in the case of tetrabetaine selenate[6], bisbetaine nitrate[7], guanidinium hydrogeselenate[8], guanidinium acrylate[9] and guanidinium perchlorate[10].

The selected spectroscopic results for mentioned above simple compounds will be shown and discussed during this lecture.

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