AB INITIO CALCULATION OF THE SULFONIC POLYSTYRENE CATION-EXCHANGER IR SPECTRUM

E. V. Butyrskaya, V. A. Shaposhnik, A. M. Butyrskii,
S. I. Karpov, L. S. Nechaeva

An optimization of the structure of the representative fragment for sulfonic polystyrene cation-exchanger in the form of cations of the alkali metals with the use of Gaussian 03 program was performed and its IR spectrum was calculated as well. Analysis of the optimized structure has demonstrated that molecules of water are incorporated between the sulfo-group and counter-ion of cation-exchanger forming hydrogen bonds between each other. It means that dissociation of the ion pair takes place. The calculated IR spectra of the representative fragment for sulpho-cation-exchanger in the range of frequencies of the valence vibrations for sulphonate group can be used as mathematical reference spectra when undertaking the analysis of this system by expert systems.