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New approach for determination of the influence of long-range order and selected ring oscillations on IR spectra in zeolites

Andrzej Mikuła[1], *Magdalena Król*[1], *Włodzimierz Mozgawa*[1], *Andrzej Koleżyński*[1]

[1]*Faculty of Materials Science and Ceramics, AGH University of Science and Technology, 30 Mickiewicza Av., 30-059 Krakow, amikula@agh.edu.pl*

Abstract:

Vibrational spectroscopy can be considered as one of the most important methods used for structural characterization of various porous aluminosilicate materials, including zeolites. On the other hand, vibrational spectra of zeolites are still difficult to interpret, particularly in the pseudolattice region, where bands related to ring oscillations can be observed. Using combination of theoretical and computational approach, a detailed analysis of these regions of spectra is possible; such analysis should be, however, carried out employing models with different level of complexity and simultaneously the same theory level.

In this work, an attempt was made to identify ring oscillations in vibrational spectra of selected zeolite structures. A series of *ab initio* calculations focused on S4R, S6R, and as a novelty, 5–1 isolated clusters, as well as periodic siliceous frameworks built from those building units (ferrierite (FER), mordenite (MOR) and heulandite (HEU) type) have been carried out. Due to the hierarchical structure of zeolite frameworks it can be expected that the total envelope of the zeolite spectra should be with good accuracy a sum of the spectra of structural elements that build each zeolite framework. Based on the results of HF calculations, normal vibrations have been visualized and detailed analysis of pseudolattice range of resulting theoretical spectra have been carried out. Obtained results have been applied for interpretation of experimental spectra of selected zeolites.

Keywords: *ab initio* calculations; zeolite; vibrational spectra; long-range ordering