Physical Properties of Metal–Organic Zeolitic Imidazolate Frameworks

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Abstract. Zeolitic imidazolate frameworks represent new materials falling into the large group of metal–organic frameworks with wide application potential. The present work is focused on the study of fundamental properties of imidazolate compound $[\{Zn(mIm)_2 \cdot 2H_2O\}_\infty]$,which is referred in literature as ZIF–8. Measurements of infrared spectra in the mid-infrared and far-infrared regions at room temperature as well as heat capacity in the range from 2 to 300 K were performed. The character of the infrared spectra suggests why the specific heat data values are so small, and even at 300 K the values are much lower than the classical value of 3sR resulting from the equipartition principle. Analysis of the specific heat of the ZIF–8 powder sample within the Debye model including only the contribution of three acoustic phonon branches revealed deviations of the model from experimental data already above 20 K. Low–frequency optical modes as indicated by infrared spectra are responsible for the observed deviations.