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The theory of hindered molecular motion and its application to spectroscopic studies

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Abstract

A stochastic theory of the classical local hindered motion of small molecules in molecular and ionic crystals is presented in detail. The so-called extended angular jump model, being intermediate between the rotational diffusion model and the model of fixed angular jumps, approximates the motion. In spite of the fact that dynamical quantities of the model do not relate to the hydrodynamic parameters of the continuous medium, the outcomes of the theory are suitable for molecular liquids. Two crystallographic point symmetries, the symmetry of the molecular motion and the site symmetry, including their distortions, are taken into account in the model. Applications of the theory to the description of NMR-relaxation rates and the homogeneous broadening of spectral lines excited by dielectric, infrared, Raman, Rayleigh and neutron spectroscopy techniques are given. The validity of the approach presented is confirmed by the experimental data performed in single crystalline and powder samples. © 2010 Taylor & Francis.

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Keywords

Angular autocorrelation function, Anisotropy, Correlation time, Crystallographic point symmetry group, Dielectric properties, Extended angular jump model, Hindered molecular motion, Incoherent neutron scattering, Infrared absorption, Line intensity, Line width