

# Angular auto-correlation functions in molecular crystals and liquids: Application to incoherent neutron scattering law

Bashirov F.

*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

---

## Abstract

The effect of the local hindered molecular motion in the incoherent neutron scattering spectra in crystals and liquids is studied theoretically on the basis of the angular auto-correlation functions symmetrized on the dynamical point groups. The extended angular jump model simulates the motion. The microscopic properties of the matter, the time scale and the point symmetry of the molecule motion as well as the site symmetry of the molecule, are taken into account with the help of the dynamical variables of the model. The incoherent neutron scattering function is anisotropic in a monocrystalline sample. The scattering function consists of elastic plus quasi-elastic components. The shape of the quasi-elastic scattering spectrum is expressed by the sum of the weighted Lorentzian curves symmetrized with respect to the non-identical irreducible representations of the molecule motion point symmetry group. The elastic part of the intensity is increased by the contribution arising from the molecule motion of the identity representation symmetry. The scattering expression related to the molecule motion symmetry of a perfect cubic group is similar to the well-known expression derived for the scattering from the spherical top molecules exhibiting rotation diffusion.

<http://dx.doi.org/10.1080/00268970150200460>

---