Monte Carlo Calculation of the Correlation Functions for Molecular Rotation – Application to NMR

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The Monte Carlo method for calculating correlation functions for the rotational motion of atoms is presented. This method applies to crystalline solids and allows the determination of the correlation functions for any model of rotating atoms, molecules or ions constituting the material of interest, if only its crystal structure is known. The presented method permits the calculation of the correlation functions for a whole block of unit cells, not only for a single group of particles. The described method can be employed to calculate correlation functions used in the theoretical description of NMR, dielectric or neutron diffraction experiments. As an example the correlation functions and NMR relaxation time T_1 of solid benzene are calculated by the Monte Carlo method for the.

Key words: Correlation Function; Monte Carlo; NMR; Relaxation.