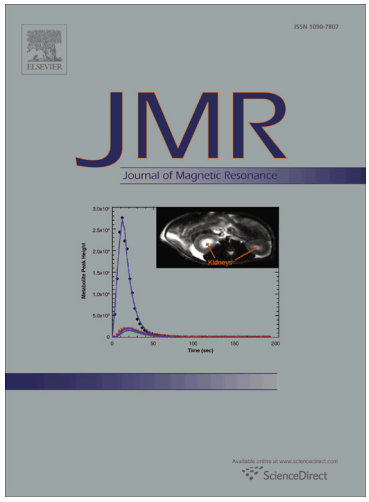

Homogeneity and EPR metrics for assessment of regular grids used in CW EPR powder simulations

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Homogeneity and EPR metrics for assessment of regular grids used in CW EPR powder simulations

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Abstract

CW EPR powder spectra may be approximated numerically using a spherical grid and a Voronoi tessellation-based cubature. For a given spin system, the quality of simulated EPR spectra depends on the grid type, size, and orientation in the molecular frame. In previous work, the grids used in CW EPR powder simulations have been compared mainly from geometric perspective. However, some grids with similar homogeneity degree generate different quality simulated spectra. This paper evaluates the grids from EPR perspective, by defining two metrics depending on the spin system characteristics and the grid Voronoi tessellation. The first metric determines if the grid points are EPR-centred in their Voronoi cells, based on the resonance magnetic field variations inside these cells. The second metric verifies if the adjacent Voronoi cells of the tessellation are EPR-overlapping, by computing the common range of their resonance magnetic field intervals. Beside a series of well known regular grids, the paper investigates a modified ZCW grid and a Fibonacci spherical code, which are new in the context of EPR simulations. For the investigated grids, the EPR metrics bring more information than the homogeneity quantities and are better related to the grids' EPR behaviour, for different spin system symmetries. The metrics' efficiency and limits are finally verified for grids generated from the initial ones, by using the original or magnetic field-constraint variants of the Spherical Centroidal Voronoi Tessellation method.

Keywords: CW EPR, simulation noise, Voronoi tessellation, regular grid, SCVT

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