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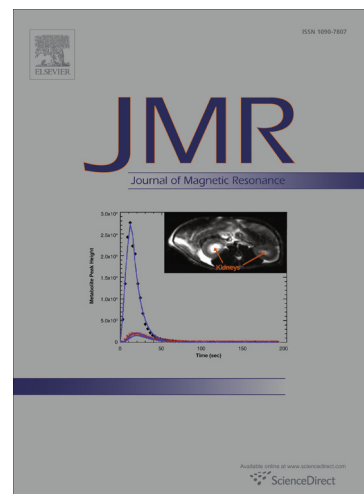
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Single-crystal NMR approach for determining chemical shift tensors from powder samples via magnetically oriented microcrystal arrays

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ABSTRACT

The single-crystal rotation technique was applied to magnetically oriented microcrystal arrays (MOMAs) of cellobiose (monoclinic) to determine the principal values and principal axes of the chemical shift tensors of C1 and C1' carbons. Rotations were performed about the magnetic χ_1 , χ_2 , and χ_3 axes of MOMA, and the measurements were taken at six different orientations with respect to the applied magnetic field. Under these rotations, crowded peaks were reduced and the peaks for the C1 and C1' carbons were identified by comparing with simulation results. Six components of the chemical shift tensor expressed with respect to the magnetic $\chi_1\chi_2\chi_3$ -frame were determined. The tensors thus obtained were transformed into those relative to the molecular frame.

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