MAR06-2005-040012

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Interference between relaxation and parameters for protein structure determination[1]

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The effect of cross-correlated relaxation on scalar and dipolar coupling measurements is analyzed. We compare one-bond proton-carbon scalar and dipolar couplings of protein methine and methylene sites obtained by monitoring proton and carbon magnetization. Apparent J-coupling constants of the same pair of nuclei vary depending on the type of magnetization involved. The discrepancies are of different magnitude for methine and methylene moieties. Dynamic frequency shifts are partially responsible for the observed differences. More importantly, the largest observed variations can be explained by processes of magnetization transfer originated by cross-correlated relaxation. These later effects are not cancelled when obtaining residual dipolar couplings.

[1]In collaboration with Nico Tjandra, National Institutes of Health.