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Separation of cross-relaxation and exchange in two-site spin systems without resolved couplings

Klochkov V., Karatayeva F., Shaikhutdinov R., Khairutdinov B., Molins M., Pons M. *Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

Abstract

Variable temperature two-dimensional nuclear Overhauser enhancement experiment (2-D NOESY) is used to extract the rate constants and cross-relaxation rates that contribute to the same cross-peaks in NOESY spectra. Rate constants (kAB) and cross-relaxation rates (RAB) for two-site spin systems are related to the ratio between the cross-peak and diagonal peak integrals (F) by the expression: RAB - kAB = $(1/2 \text{ tm})\ln[(1 - F)/(1 + F)]$, where tm is the mixing time. As a model, we investigated the exchange processes in a system of dimer calix[4]arenes of C4v symmetrical configuration with guest inclusion (benzene or benzene-d6), where the measurement of exchange processes is hindered by the presence of strong nuclear Overhauser enhancement between protons in adjacent aromatic rings in the cone conformation of the calix[4]arene.