



15N-CPMAS-NMR spectroscopy of 15N-labeled sulfadiazine/humic acid complexes

Anne E. Berns, Herbert Philipp, and Hans-Dieter Narres

Forschungszentrum Juelich GmbH, IBG 3, Juelich, Germany (a.berns@fz-juelich.de, +49-2461-612518)

The veterinary pharmaceutical sulfadiazine (SDZ) is a widely used antibiotic in intensive livestock production. A large part (up to 40 %) of such sulfonamides is eliminated as active parent with the excretions and hence reaches agricultural soils through grazing livestock and/or through the spreading of manure. Detailed knowledge on the fate of sulfadiazine in soil is essential to assess its environmental risk.

Binding and release of a xenobiotic and its metabolites in soil is mainly determined by the type of interaction with soil components like organic matter or the mineral phase. Nuclear magnetic resonance (NMR) can be used for the characterization of bound residues as binding of the xenobiotic, or its metabolites, to the soil matrix causes shifts in the initial positions of the NMR signals of the compound.

15N-CPMAS-NMR spectroscopy was applied to study the interactions between 15N-labeled SDZ and soil organic matter in the presence/absence of the natural enzyme laccase. Through the use of synthesized model compounds, we identified the sequestration of parent and metabolite, the formation of covalent amide bonds and of Michael-type additions to chinoid systems. Furthermore, we hypothesize the presence of van der Waals interactions and hydrogen bridging.