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The combined use of quantum chemical calculations and CP/MAS NMR spectroscopy to investigate soil bound residues of labeled xenobiotics

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Application of solid state Nuclear Magnetic Resonance (NMR) spectroscopy to 13C- and 15N-labeled compounds is a powerful tool to study the interactions of xenobiotics with soil and its components. The type of interaction with soil components, like organic matter or the mineral phase, influences binding and release of a xenobiotic and its metabolites in soil. As such interactions to the soil matrix cause shifts in the initial positions of the NMR signals of the investigated labeled compound, NMR can be used to elucidate the binding type of bound residues.
Density functional theory (DFT) calculations are excellent suited to support such NMR studies of xenobiotics. In a first step, DFT calculations were used to support the interpretation of the spectra of labeled xenobiotics, their metabolites and reaction products synthesized through reaction with model substances (representing specific functionalities of humic substances). In a second step, they allow to evaluate the influence of possible bonds on the initial chemical shift (e.g. towards higher or lower field). This can be especially helpful in the case of bonds like van-der-Waals interactions, for which it is difficult to prepare defined model substances.
CP/MAS-NMR spectroscopy and DFT calculations were applied to study the interactions of several labeled xenobiotics and soil organic matter.