Evaluation of abiotic and biotic ethylene dibromide transformation using dual C and Br isotope analysis

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Over the last decades, concepts involving compound specific stable isotope analysis (CSIA) have been developed allowing the qualification and quantification of *in situ* (bio)transformation and evaluation of the related reaction mechanisms of transformation of common groundwater contaminants such as the chlorinated ethenes but also pesticides such as γ-hexachlorocyclohexane (Lindane). Brominated subtances are present in the environment as well either from natural or anthropogenic sources and have applications e.g. as flame retardants or biocides. Compared to their chlorinated analogues, however, the transformation pathways of these brominated substances are largely unknown and concepts to assess their fate *in situ* are absent.

Therefore, we investigated the isotope effects for both carbon and bromine during transformation using ethylene dibromide (EDB), a fumigant and pre-cursor for chemical synthesis, as model compound. EDB transformation was tested under alkaline conditions; by reduction with Zn0, reduced corrinoids or by *Sulfurospirillum multivorans;* during aerobic degradation by *Ancylobacter aquaticus* as well as oxidation by Fenton reagent. The resulting isotope effects correlated with the presumed reaction types based on observed reactivity for 1,2-dichloroethane: dehydrobromination, dihaloelimination, nucleophilic substitution and oxidation by hydroxyl radicals. Calculated apparent kinetic isotope effects (AKIE) carbon fit with expected values for the reaction types, however, bromine AKIE exceeded the theoretical values. In summary, our study confirmed that CSIA may be used for both the evaluation of *in situ* transformation as well as to distinguish different degradation pathways.