**Compound specific and enantioselective stable isotope analysis as tool to monitor transformation of hexachlorocyclohexane (HCH) in aquifers**

YAQING LIU†\*, SAFDAR BASHIR#\*,REINER STOLLBERG†,RALF TRABITZSCH†,HEIDRUN PASCHKE$, IVONNE NIJENHUIS†, HANS-HERMANN RICHNOW†.

†Department of Isotope Biogeochemistry, Helmholtz Centre for Environmental Research-UFZ, Permoserstraße 15, 04318 Leipzig, Germany

†Department Groundwater Remediation, Helmholtz Centre for Environmental Research-UFZ, Permoserstraße 15, 04318 Leipzig, Germany

$Department of [Analytical Chemistry](http://www.ufz.de/index.php?en=1442), Helmholtz Centre for Environmental Research-UFZ, Permoserstraße 15, 04318 Leipzig, Germany

#Current address: University of Agriculture Faisalabad, Institute of Soil & Environmental Sciences, Faisalabad, Pakistan

\*Co-first author

Hexachlorocyclohexane (HCH) isomers and enantiomers are pollutants of particular concern because of their widespread distribution in the environment, toxicity and persistence. The production and application of HCHs started in early 1950s and resulted in contamination of soil and aquifers. Only γ-HCH (Lindane) has pesticidal activity. The purification of Lindane resulted in the production of other waste isomers which were mostly dumped near the production sites. The local chemical industry in Bitterfeld-Wolfen, Germany, produced Lindane from 1951 to 1982 which resulted in contamination of soils and aquifers.

HCH contaminated plumes have been developed in the groundwater aquifers down gradient the HCH production and the dump site in Bitterfeld. For the evaluation of the degradation in the aquifer, compound specific and enantiomer specific carbon stable isotope analysis were applied as tool for the investigation of *in situ* transformation of HCH. The concentrations and carbon stable isotope composition of HCH isomers and enantiomers of α-HCH were investigated as indicators for *in situ* transformation.

Sampling campaigns were performed in 2013 and 2014, where more than 40 groundwater samples were collected from the generally anoxic aquifers (DO:<0.7mg L-1) with pH values between 3 to 7. Additionally, samples from historical production as well as muck samples from a dump site were used as representative for original production. In more than a quarter of the wells HCH isomers were detected, where the δ-HCH dominated with a concentration up to 264µg L-1 for a single isomer. At the same time, in most wells the α-HCH was detected with a concentration up to 242µg L-1.

Compared to the isotope signatures of muck samples, carbon isotope discrimination (Δ=δ13Cwell-δ13Cmuck) was up to 5.3‰ in water samples. The enrichment of carbon stable isotope composition of HCH isomers in several investigated wells suggested transformation of HCHs. Furthermore, the carbon isotope value of selected HCH was enriched along the presumed flow direction. The enantiomer fraction (EF) was shifted up to 0.35 suggesting biodegradation, interestingly also in the well with pH 3.4. Comparing EF and carbon isotope signatures to literature data, a biodegradation could be concluded based on the shift in EF. Determination if this biodegradation was aerobic or anaerobic would require further reference experiments or additional approaches, such as molecular biology, for detection of key degrading microorganisms.