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Transformation of Geogenic Iodine Species in Aquifer Systems: Molecular Constraints by Organic Matter

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Dissolved organic matter (DOM) plays a pivotal role in regulating hydro-biogeochemical processes and contaminant behavior in groundwater systems. High-iodine groundwater is recognized as a major type of geogenic contaminated groundwater, posing a global threat to water security comparable to that of arsenic- or fluoride-contaminated groundwater. The environmental complexity of iodine arises from its species. In aquifers, iodine typically exists as iodate, iodide, and organic iodine (OI), which differ markedly in toxicity and mobility. Among these species, OI exhibits higher toxicity than inorganic iodine. Mobility controls their enrichment in groundwater, with iodide dominating in groundwater, while OI and iodate preferentially accumulate in sediments. Therefore, understanding iodine transformation among different species is critical for evaluating its toxicity, mobility, and environmental risk in aquifers. However, the molecular properties of OI, the mechanisms underlying DOM iodination responsible for OI formation, and their coupling with hydro-biogeochemical processes remain poorly understood and are strongly influenced by their respective molecular characteristics. Focusing on the Jianghan Plain, a region characterized by widespread high-iodine groundwater, we combined field investigations, Fourier transform ion cyclotron resonance mass spectrometry, and controlled incubation experiments to elucidate the dynamics of iodine, especially OI. Specifically, this research aims to: (1) characterize the molecular composition of OI within groundwater systems; (2) unravel molecular-scale transformation pathways from inorganic iodine to OI; and (3) clarify molecular fractionation among transformation pathways and its subsequent impacts on the geochemical behavior, mobility, and retention of OI under aquifer conditions. Preliminary results indicate the OI in groundwater systems are mainly composed of highly unsaturated compounds and aromatics. The transformation of inorganic iodine to OI is primarily dominated by the addition reaction (47.0%) and followed by substitution reaction (33.8%). Notably, addition reaction during iodination processes substantially enhances affinity of OI for Fe oxides by increasing oxygen-containing functional groups. These findings provide new molecular-level insights into the transformation mechanism of iodine species in aquifer systems.