A holistic view of organic sulfurization

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Sulfurization, the interaction of inorganic sulfur with the plethora of organic molecules in natural systems to form a fingerprint of organosulfur compounds, is critical in considering the formation and clean use of fuels, metal mobility, and the global cycling of carbon through time. A series of experiments were executed to determine the detailed organosulfur signatures associated with reactivity of sulfide, polysulfide, thiosulfate, sulfite, and sulfate with two different dissolved organic matrices. We utilized X-ray near-edge adsorption structure spectroscopy (XANES) and Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS), giving us a look at thousands of different molecules in a single sample. Sulfur speciation was defined using a combination of electrochemical and chromatographic techniques, and indicate sulfurization is coeval with oxidation of reduced sulfur forms by organic molecules. Results show for the first time that significant sulfurization is possible with the more oxidized sulfur species thiosulfate and sulfite, and that each sulfur intermediate yields distinctly different patterns of organic sulfur molecules formed. We utilize these experiments to give us additional insight on relatively fast organic sulfurization occurring in hydrothermal and meromictic lakes where we have consistent FTICR-MS and sulfur speciation information.