Analysis of mixed selenium-sulfur compounds in waters by electrospray-Fourier transform-ion cyclotron resonance-mass spectrometry

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Selenium (Se) is of high environmental concern at many industrially-impacted sites across North America, due to its potential to accumulate in aquatic food chains, and cause negative developmental effects in top predators, such as game fish and water fowl. It is well established that the environmental fate and ecotoxicity of Se depend strongly on its speciation, and that, due to its chemical similarity to sulfur (S), Se forms a wide variety of mixed soluble compounds in waters containing reduced S species. It is obvious that this should impact Se speciation in certain industrial and environmental waters, yet to date only one mixed Se-S species, selenosulfate, has been identified in such waters.

The three main limitations in the study of soluble Se-S species in waters are 1) the absence of commercially-available standards, 2) the instability of such compounds towards oxidation and 3) problems associated with the unequivocal mass spectrometric identification of such compounds with nominal resolution electrospray-mass spectrometry (ES-MS), e.g. using commonly available triple quadrupol instruments. The last problem relates to the fact that is it sometimes difficult to distinguish between compounds containing both S and oxygen (O) atoms in molecules with unknown number of atoms (besides Se atoms).

In this study, I will demonstrate the use of Fourier transform-ion cyclotron resonance-mass spectrometry (FT-ICR-MS) with electrospray sample introduction for the improved identification of unknown mixed Se-S species in waters. This MS approach achieves spectral resolution well above 10^6 and thus allows direct determination of the number of O, S and Se atoms in a molecule via the abundance of isotopic satellites. This method was applied to the determination of soluble Se-S species in reaction mixtures of Se species with reduced S species. Results for different reaction mixtures, reaction times and reaction conditions will be presented and discussed in terms of their applicability to environmental and industrial waters.