Contribution ID: **29** Type: **Oral**

Analysis of EXAFS spectra with the aid of neural networks: Aqueous U(VI) complexes with aliphatic (hydroxy-) carboxylic acides

Thursday 22 May 2014 11:55 (25 minutes)

Sixty U LIII-edge EXAFS spectra from 13 structurally different aliphatic ((di-)hydroxy-) carboxylic acids (acetic, succinic, tartaric, lactic, 3-hydroxybutyric, citric, formic, malic, maleic, malonic, oxalic, propionic, and tricarballylic acid) were measured at different pH, uranium and ligand concentrations. Each of the ligands can form several metal complexes, which may coexist as mixtures depending on the physicochemical parameters (pH, concentration).. The ligands were chosen in such a way that they would allow a structural analysis of the complexes solely by using the exclusion principle, i.e. by comparing the spectra with respect to pH, concentration, presence/absence, number, position and the type of the functional group/s. Due to the high number of different constellations in this highly correlated system, simple inspection by eye and other conventional tools will possibly lead to different solutions and is therefore prone to misinterpretation. Artificial neural networks, such as self-organizing maps (SOM), are expected to be better adapted and more specialized for dealing with such highly complex systems. We show that the inclusion of the Beer-Lambert law, in the training period of SOM, leads to a new kind of supervised learning algorithm [1] which enables the determination of the spectra and fractions of the different U(VI) complexes. Moreover, we show that the new SOM algorithm allows the inclusion of available information such as the ligand structures and the physicochemical parameters so that latent relationships between them and the spectra of the complexes are revealed.

[1] Domaschke, K. et al. (2014) Proceedings of ESANN.

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Session Classification: Theoretical and Modeling Tools

Track Classification: Theoretical and Modeling Tools