

Detection and assignment of aqueous inorganic Fe-polymers by mass spectrometry (TOF MS)

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Some phases, such as Fe oxyhydroxides and oxyhydroxysulfates, have become a controversial topic of discussion due to their undefined structure, their properties or even their formation processes. Among them, schwertmannite is one of the most extended low crystalline Fe-phases. It is easily found in acid drainage (AD) systems. Even though it has been largely studied, final models of its formation or structure have not been found yet¹.

Electrospray ionization source (ESI) coupled to an analyser by time of flight (TOF) mass spectrometry is an analytical technique that has been largely used in organic chemistry, but there are not many works where it has been applied to the study of inorganic polymers in aqueous environments².

In this work, ESI-TOF analyses have been performed in order to find out the evolution of Fe-polymers enrolled in a possible non-classical nucleation and growth of schwertmannite. In this process, two different synthesis methodologies have been followed: heating a $\text{Fe}_2(\text{SO}_4)_3$ solution at different temperatures and Fe oxidation (from an initial $\text{Fe}(\text{SO}_4)$ solution) by adding H_2O_2 . Most of the identified polymers appear in both experiments, and big polymers disappear from solution when precipitates are formed. A data base of the identified polymers (cationic and anionic) has been created.

¹Fernandez-Martinez, A., Timon, V., Romaman-Ross, G., Cuello, G. J., Daniels, J. E., & Ayora, C. (2010). *Am. Min.*, 95, 1312–1322.

²Sarpola, A., Hietapelto, V., Jalonen, J., Jokela, J., & Laitinen, R. S. (2004). *J. of Mass Spectrom.*, 39(4), 423–430.