

Detection of inorganic polymers involve in hydrobasaluminite synthesis by mass spectrometry

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Inorganic polymers in aqueous solutions are being regarded as essential components in new theories concerning non-classical nucleation and growth of nanominerals relevant to environmental nanogeosciences¹. The study of those complex natural processes requires multi-technique analytical approaches able to characterize the solutions and their constituents (solutes, oligomers, polymers, clusters and nanominerals) from in different scales. A novel analytical approach involving an electrospray ionization source (ESI) coupled to time-of-flight mass spectrometry (TOF/MS) was developed to identify inorganic polymers in aqueous solution. To this end, the presence of initial Al oligomers and their polymerization processes was studied during a nanomineral aqueous synthesis (hydrobasaluminite, $\text{Al}_4\text{SO}_4(\text{OH})_{10} \cdot 12\text{-}36\text{H}_2\text{O}$). Ensuring the feasibility and robustness of the methodology, a meticulous study of the ESI-TOF MS working conditions was performed. For the first time in the study of inorganic polymers in the Earth sciences, the mass accuracy error (ppm) has been reported and the use of significant decimal figures of the m/z signal has been taken into account. Complementary to this, a four step polymer assignment methodology and a database with the Al^- and Al-SO_4^{2-} polymers assigned were created.

¹G.I. Yucelen, R.P. Choudhury, A. Vyalikh, U. Scheler, H.W. Beckham, S. Nair, U. States. (2011) J. Am. Chem. Soc. 133, 5397–5412.