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A spectroscopic study of the complexation reaction of trivalent lanthanides with a synthetic acrylate based PCE-superplasticizer

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Abstract

The interaction between different trivalent lanthanides and a synthetic acrylate based PCE-superplasticizer (52IPEG4.5) is investigated by using a combination of laser- and synchrotron based spectroscopic techniques. Time-resolved laser fluorescence spectroscopy (TRLFS) is used to obtain thermodynamic data (stability constants (log β'(T), reaction enthalpy ($\Delta_r H$) and entropy($\Delta_r S$)) of the complexation reaction of Eu(III) and 52IPEG4.5 as a function of the temperature (20 - 80 °C) and ligand concentration (< 2 g/kg) in 0.1 mol/kg NaCl solution. Under the chosen experimental conditions, the increase in temperature mainly affects the complexation properties (loading capacity) of the macromolecule itself rather than the stability constant of the formed complex (log β'(T) ranging between 6.5 - 5.9). The thermodynamic results are complemented by extended X-ray absorption fine structure (EXAFS) spectroscopic measurements to resolve the molecular structure of 52IPEG4.5 complexes with Eu(III), Gd(III), and Tb(III). The results show, that each metal ion is coordinated by three carboxylic groups within the 52IPEG4.5 complexes. Furthermore, the determined interatomic distances exhibit that the functional groups are attached in a bidentate end-on fashion.

Keywords: EXAFS, TRLFS, Geochemistry, Thermodynamics, Nuclear Waste Disposal, Coordination Chemistry

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