A new approach to determination of hydration equilibria constants for the case of $[Er(EDTA)(H_2O)_n]^-$ complexes.

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Streszczenie

Two anionic complexes [Er(EDTA)(H2O)2](-) and [Er(EDTA)(H2O)3](-) were obtained in the form of the following compounds: [C(NH2)3]2[Er(EDTA)(H2O)2]ClO4·6H2O () and Na[Er(EDTA)(H2O)3]·5H2O (), respectively. The UV-vis-NIR absorption spectra of both monocrystals were measured at room temperature and at 4.2 K. The influence of the coordination number changes on intensities of the f-f transitions and the crystal field splitting of (2S+1)LJ multiplets are discussed. The weighted sum of molar absorption coefficients of f-f transitions in the spectra of and was used to reproduce the absorption bands of the Er(3+)-EDTA complex in aqueous solution. This approach allowed us to estimate that the complex in solution exists in 95% as the 8-coordinate [Er(EDTA)(H2O)2](-) species and in 5% as the 9-coordinate [Er(EDTA)(H2O)3](-) ones as well as to calculate the conditional hydration equilibrium constant (Kaqua) of the reaction: [Er(EDTA)(H2O)3](-) ↔ [Er(EDTA)(H2O)2](-) + H2O which is rather difficult to determine by using other methods. The Kaqua value was found to be 19 ± 1.

Adres publiczny

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Strona internetowa wydawcy

https://www.rsc.org/