

The ab initio and experimental study of the spectroscopic and magnetic properties of Ho(III)-EDTA

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In this paper the ab initio calculations of the electronic structure and the magnetic properties are discussed in the context of the experimental data for the Ho–EDTA complex. In the calculations different models of the cluster have been applied to examine the influence of various parts of the environment of the Ho(III)-EDTA complex on its properties. In particular, the calculations support the expectation that the presence of the water molecules in the first coordination sphere has considerable impact on the oscillator strengths of the electronic transitions and the magnetic susceptibility of the material under study. We have reconsidered the effect of the dynamical electron correlation on the magnetic susceptibility.

Słowa kluczowe

Lanthanide elements, Magnetic properties, Electronic structure calculations, UV-vis-NIR spectroscopy

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