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# Crystal structure and absorption spectroscopy of $Ln(HF_2CCOO)_3{\cdot}3H_2O$(Ln=Pr,Er) single crystals.

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Streszczenie

Crystal structures of $Ln(HF_2CCOO)_3{\cdot}3H_2O$ (Ln=Pr, Er) compounds were determined by X-ray analysis. Both crystals proved to be isomorphous. They are triclinic, space group with $\alpha$=66.60(2)°, $\beta$=79.34(2)°, $\gamma$=77.74(2)° and $Z$=2 for the Pr compound and $\alpha$=66.90(2)°, $\beta$=79.34(2)°, $\gamma$=77.80(2)° and $Z$=2 for the Er one. The Ln(III) ion adopts an 8-coordinate geometry with six oxygen atoms from carboxylate groups and two oxygen atoms from water molecules, which is best described as the best slightly deformed square antiprism. Absorption spectra of the $Pr(HF_2CCOO)_3{\cdot}3H_2O$ single crystal were measured at room and low temperatures. Intensities of the f–f transitions were analysed on the basis of the Judd–Ofelt theory. The results for the praseodymium difluoroacetate single crystals are compared to those for the lanthanide trifluoroacetates monocrystals. Vibronic mechanism of 4f–4f transitions is discussed.

Słowa kluczowe

Crystal structure, Electronic spectra, Lanthanide difluoroacetate complexes, Vibronic mechanism

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