

Optical properties and crystal structure of lanthanide(III) coordination compounds with 2-propenoic acid.

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Coordination compounds of a new type, $\text{Ln}(\text{C}_3\text{H}_3\text{O}_2)_3 \cdot x\text{H}_2\text{O}$ (where $\text{Ln} = \text{Nd}^{3+}$, Dy^{3+} ; $\text{C}_3\text{H}_3\text{O}_2^-$ = 2-propenoic anion/acrylic anion, $x = 3$ or 1.5 for Nd and Dy, respectively), were obtained in crystalline state and their structures were determined. Both crystals are composed of polymeric chains and in both crystals there are two symmetry-independent lanthanide ions, each with a different coordination sphere. The Nd crystal (**I**) is monoclinic, space group $P2_1/c$, and the Dy crystal (**II**) is triclinic, . The Ln^{3+} ions occupy low-symmetry sites in the dimeric structure of $\text{Ln}(\text{H}_2\text{CCHCOO})_3 \cdot x\text{H}_2\text{O}$. The spectroscopic investigations of the title monocrystals at room and low temperatures down to 4.2 K were performed to explain the electrostatic nature of the Ln^{3+} -ligand bond. Variations in the spectroscopic parameters and their correlations with the nature of the Ln^{3+} -L bond are discussed. Analysis of the low-temperature spectra indicates the presence of ion-pair interactions. The influence of the $-\text{CC}-$ double bond in the substituent of the carboxylate ions on the distribution of charge, polarity, strength, and character of the $\text{Ln}-\text{O}(\text{L})$ coordination bond is analysed. The number of electronic components observed in the absorption spectra measured at 4.2 K is compatible with that expected for these systems. Spectroscopic measurements allowed us to compare the optical properties of $\text{Ln}(\text{H}_2\text{CCHCOO})_3 \cdot x\text{H}_2\text{O}$ with lanthanide acetates and other carboxylates.

Słowa kluczowe

lanthanides, 2-propenoic acid, Acrylic acid, UV-Vis spectroscopy, X-ray diffraction

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