

Correlation between spectroscopic characteristics and polymeric structure of Er^{3+} complex with pent-4-ynoate.

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A coordination compound of an Er^{3+} with pent-4-ynoate was obtained in crystalline state and its structure was determined. The compound is a carboxylate-bridged one-dimension polymeric complex consisting of two types of chains differing in the coordination number (CN) of Er(III) and the number of water molecules coordinated to the metal. One of the chains contains an Er^{3+} ion having CN = 8 when one water molecule is present in its coordination sphere or CN = 9 when water is bonded to Er too. The other chain contains Er with CN = 8, but only one metal cation contains one water molecule in its coordination sphere. Each pent-4-ynoate ligand chelates one metal ion and bridges to the next metal ion. Consequently, all coordination bonds of Er(III) , except those with water oxygen, are due to O atoms from carboxylate groups. The structure of the compound was determined by single crystal X-ray analysis. The compound crystallizes in a monoclinic system with space group $P2_1/a$ and the following unit cell parameters: $a = 15.912(4)$, $b = 10.517(3)$, $c = 41.488(12)$ Å, $\beta = 99.84(3)^\circ$, $V = 6841(3)$ Å³, $Z = 4$. Spectroscopic investigations at room and low temperatures were performed in order to understand the electrostatic nature of the Ln^{3+} –ligand bonds. The effect of the CC triple connection in carboxylate ions on the distribution of charge, polarity, strength, and character of the LnO(L) coordination bond was analyzed.

Słowa kluczowe

lanthanides, Erbium, Pent-4-ynoate, X-ray diffraction, UV–Vis spectroscopy

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