

Structural and spectroscopic studies of neodymium complexes with S(+)-mandelic acid.

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Streszczenie

The crystal structure of tetraquaahexakis-S(+)-mandelatodineodymium trishydrate was determined by the X-ray diffraction method. The compound crystallizes in the monoclinic space group $P2_1$ with the following unit cell parameters: $a = 10.536(2)$, $b = 16.089(3)$, $c = 15.316(3)$ Å, $\beta = 97.96(2)^\circ$. The structure consists of polymeric $[\text{Nd}_2(\text{Man})_6(\text{H}_2\text{O})_4 \cdot 3\text{H}_2\text{O}]_\infty$ chains (where $\text{ManH} = \text{S}(+)\text{-2-hydroxy-2-phenylacetic acid}$ or $\text{S}(+)\text{-mandelic acid}$), with two symmetry independent Nd^{+3} ions. Both neodymium ions are nine-coordinate but differ in their environments. $\text{Nd}(1)$ is surrounded by two water molecules, five carboxylate and two hydroxyl oxygen atoms, $\text{Nd}(2)$ is coordinated by two water molecules, four carboxylate and three hydroxyl oxygen atoms. Crystals of neodymium mandelate complex were characterized by thermal analysis as well as by IR and UV-vis-NIR absorption spectroscopy.

Słowa kluczowe

neodymium, mandelic acid, X-ray structure, UV-vis-NIR-IR spectroscopy, rare earths

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