Lanthanide carbonates.

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Streszczenie

The crystal and molecular structures of the rare earth carbonates with the general formulae [C(NH2)]3[Ln(CO3)4(H2O)]·2H2O (where Ln = Pr3+,Nd3+,Sm3+,Eu3+,Gd3+,Tb3+)and[C(NH2)]3[Ln(CO3)4]·2H2 (where Ln = Y3+,Dy3+,Ho3+,Er3+,Tm3+,Yb3+,Lu3+) were determined. The crystals consist ofmonomeric [Ln(CO3)4(H2O)]5–or [Ln(CO3)4]5–complexanions in which the carbonate ligands coordinate to the Ln3+ion in a bidentate manner. The spectroscopic (UV/Vis/NIRand IR) properties of the crystalline lanthanide carbonates,as well as their aqueous solutions, were determined. Corre-lation between the spectroscopic and the structural data en abled us to conclude that the [Ln(CO3)4(OH)]6–and [Ln-(CO3)4]5–species predominate in the light and heavy lantha-nide solutions, respectively. The nature of the Ln–O interac-tion was also discussed. The experimental data, as well asthe theoretical calculations, indicated that the Ln–O(CO32–)bond is more covalent than the Ln–O(OH2) bond. Moreover,the covalency degree is larger for the heavy lanthanide ions.Inspection of the NBO results revealed that the oxygen hy-brids, with the approximate composition sp4, form stronglypolarized bonds with the 6s6p5d4hybrids of lutetium

Słowa kluczowe

structure elucidation, UV-vis, NIR spectroscopy, IR spectroscopy, density functional calculations

Adres publiczny

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