Versatile binding modes of chiral macrocyclic amine towards rare earth ions.

Autorzy

Karol Wydra

Michał J. Kobyłka

Tadeusz Lis

Katarzyna Ślepokura

Jerzy Lisowski

Rok wydania

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Depending on the reaction conditions, the enantiopure macrocycle H_3L containing three phenolic units is able to form mono- and trinuclear coordination compounds with rare earth metal ions. In these complexes this macrocycle can act as protonated H_4L^+, neutral H_3L, monodeprotonated H_2L^-, bis-deprotonated HL^{2-} or tris-deprotonated L^{3-} ligand. X-ray crystal structure of the Y(III) derivative of the protonated macrocycle shows highly folded conformation of the ligand with N_2O_3 set of donor atoms, while the structure of the Y(III) complex of the monodeprotonated macrocycle shows more regular helically twisted conformation of the ligand. Under basic conditions trinuclear complexes of the type $[M_3L(OH)_2]$ are formed with most of rare earth ions, where the macrocycle acts as N_6O_3 ligand. This type of complex is not formed for the La(III) and Ce(III) ions of the largest radii within the lanthanide(III) series, instead trinuclear complexes of the type $[M_3L_2]$ are formed. The X-ray crystal structures of La(III) complex with fully deprotonated or bis-deprotonated macrocycles indicate that each macrocyclic unit binds only two metal ions, while one of them is shared by two macrocycles.

Słowa kluczowe

Rare earths, Macrocycles, Chiral ligands, Coordination chemistry, Structure elucidation

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