Abstract

Macrocyclic complexes are of great interest due to their utilization in many medicinal applications, such as MRI contrast agents and radiopharmaceuticals. These complexes overcome the toxicity of free heavy metal ions and, thus, enable their use *in vivo*. In this Thesis, diamide derivative of DOTA (*t*DODAM) and its lanthanide(III) complexes were prepared and characterised in solution and in the solid state. For cerium(III) complex, formation and dissociation kinetics were studied. Structure and dynamics of europium(III) complex were investigated by multinuclear NMR spectroscopy and various 2D NMR techniques. Similarly to Ln(III)-DOTA complexes, the complexes form square-antiprismatic (SA) and twisted-square-antiprismatic (TSA) isomers and their ratio in solution was determined across the lanthanide series. Structures of 7 lanthanide(III) complexes in the solid state were determined. Thermodynamic data were obtained for Cu(II), Zn(II), Pb(II), Ce(III), Eu(III) and Lu(III) complexes by potentiometric titration.