

Title: Macrobicyclic ligands for use in MRI

Author: Bc. Miroslav Pniok

Department: Department of Inorganic Chemistry, Faculty of Science

Supervisor: doc. RNDr. Jan Kotek, Ph.D.

Supervisor's e-mail address: modrej@natur.cuni.cz

Abstract: The aim of this project is to synthesize new kind of macrobicyclic ligands for Ln^{3+} ions, especially Gd^{3+} ion. Gadolinium(III) complexes are widely used in the clinical practice as contrast agents for MR imaging and an improvement of their properties is in the center of interest of many scientific teams. The macrobicyclic ligands have been designed to make possible coordination of two water molecules in the first coordination sphere with fast water exchange. The macrocyclic core (cyclen) is combined with a linking phosphinate chain in N^1, N^4 - and N^1, N^7 -positions forming a cryptand-like structure. The N^1, N^7 -isomer Et_2L^1 was synthesized in a small amount so only the N^1, N^4 -isomer H_2L^3 has been studied. The protonation constants have been determined by pH ^{31}P NMR titration.

Keywords: cyclen, chelating agent, cryptand, MRI, phosphinate