Relaxometric, Thermodynamic and Kinetic Studies of Lanthanide(III) Complexes of DO3A-based Propylphosphonates

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Development of the responsive probes is one of the most exciting topics in the contrast agent research. Design of the pH sensitive probes, for example, can be an important issue in the early cancer diagnostic and formation of pH maps.[1] This can be reached by introduction of different functional groups such as phosphonates at the fourth nitrogen of the DO3A molecule. [2] Two DO3A-based ligands and their Gd^{3+} and Eu^{3+} complexes containing ethyl-protected and unprotected propylphosphonates in the side chain were investigated. Proton relaxometric *in vitro* studies at 20 MHz and 60 MHz and 37 °C of the Gd^{3+} complex containing free acid exhibited relative changes of up to 56% in r_1 relaxivity when the pH of the medium was changed from 4 to 7. This change is explained by the increase in the number of coordinated water molecules from 1 to 2. Temperature dependent relaxivity and NMRD profiles of Gd^{3+} complexes showed a slightly increased rotational correlation time, which is characteristic of phosphonate-containing compounds. Thermodynamic and kinetic studies of the Gd^{3+} and Eu^{3+} complexes were performed by means of potentiometry and luminescence spectroscopy. The results indicate that the thermodynamic stability and kinetic inertness of these complexes are sufficient for their *in vivo* application.

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