

Abstract

Abstract: Contrast agents for magnetic resonance imaging frequently employ organic complexes of paramagnetic ions. The present work studies rotation of phosphonate group in Ln^{III} complexes of monoethylester-P of 1,4,7,10-tetraazacyclododecane-4,7,10-tris(karboxymethyl)-1-methylphosphonic acid ($\text{Lndo3ap}^{\text{OEt}}$), specifically $\text{Lado3ap}^{\text{OEt}}$ and $\text{Cedo3ap}^{\text{OEt}}$. ^{31}P and ^1H NMR spectra were measured in a wide temperature range. Transverse relaxation times and chemical shifts of the two ^{31}P spectral lines which undergo mutual chemical exchange were estimated. The phosphorus spectra were then subjected to line-shape analysis, thus characterizing the chemical exchange connected to phosphonate rotation. This process yielded temperature dependence of both rate coefficients and relative populations between the two diastereoisomers for both studied molecules. The thermodynamic parameters were obtained and compared with similar complexes with phosphonate rotation. The knowledge of the detailed kinetics can later lead to improvements of the efficiency of the contrast agents.

Keywords: nuclear magnetic resonance, MRI contrast agent, kinetics of conformational exchange