Effect of Mg and Ca on the stability of the MRI contrast agent Gd–DTPA in seawater

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Gadolinium diethylenetriaminepentaacetic acid (Gd–DTPA) is widely applied as a contrast enhancer in medical MRI. It combines the unique magnetic properties of Gd with the extreme stability of the DTPA complex, allowing it to be completely excreted from the body within hours of being administered, without releasing toxic Gd^{3+} ions. As Gd–DTPA is not captured in wastewater treatment plants (WTPs), concentrations in rivers have increased globally by orders of magnitude following its introduction in 1987, whence it is now used as a conservative tracer of WTP effluents and aquifer recharge. The complex seems impervious to estuarine scavenging and is beginning to emerge in coastal waters, yet it is unknown how its stability is changed by competition for the DTPA ligand from major seawater cations.

We performed potentiometric titrations at seawater ionic strength (0.7 M $NaClO_4$) to determine dissociation constants of the five DTPA carboxylic acid groups, as well as stability constants of Mg, Ca, and Gd complexes with the fully deprotonated and single-protonated ligand. These are in general agreement with literature values at low ionic strength and confirm that complexes with Ca are more stable than with Mg. A side-reaction coefficient for trace-metal-free seawater, calculated from these results, suggests that Gd–DTPA may be significantly destabilized in coastal waters by competition from Mg and Ca ions, causing dissociation and release of as much as 15% of the organically complexed Gd from the ligand. Some implications for accumulation of Gd in the marine environment and the need to further study the environmental fate of this contaminant will be discussed.