
Building a consistent thermodynamic database for gadolinium inorganic complexes in aqueous solution

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Among the so-called Technology-Critical Elements (TCEs), gadolinium occupies a special place because it is the TCE with higher concentration increase in continental surface waters. The main reason is its use as contrast agent in Magnetic Resonance Imaging (MRI) due to its paramagnetic properties [1]. Because of gadolinium toxicity as free metal ion, it is administered as a chelate with a strong complexing organic molecule. These chelates are not retained in water treatments plants. However they are sensitive to UV radiations and anaerobic treatments [2].

It is therefore important to understand its behaviour in both biological fluids and natural environmental compartments. In this context, thermodynamic modelling is a useful tool, but requires an extensive knowledge of the solution chemistry of the element.

We have performed a comprehensive compilation of existing equilibrium constant values for gadolinium inorganic complexes. Once all published values collected, they have been uploaded in JESS (http://jess.murdoch.edu.au/jess_home.htm) and the 'best' set of equilibrium constants calculated following the embedded approach. Fewer original data than initially estimated exist, with a lot of 'reuse' of old equilibrium constant values even in recent studies.

References

- [1] C. Olchoway *et al.*, *PLOS ONE*, **12**, e0171704 (2017)
- [2] D. Clases *et al.*, *TrAC Trends in Analytical Chemistry*, **104**, 135-147 (2017)