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Gin-ya Adachi



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Proposal of the logarithm partial stability constant (PLSC) and its application to rare earth diethylenetriamine-N,N,N',N',N"-pentaacetic acid (DTPA) complexes

Gin-ya Adachi

Osaka University, Private Office, 32-29, Mikage 2chome, Higashinada, Kobe, 658-0047, Japan
gadachi@fj8.so-net.ne.jp

Abstract: The purpose of this article is to propose the idea of “a partial stability constant” for the complex formation of polyamine polyacetic acids with tripositive rare earth ion. Each coordinating group has its own characteristic stability constant, i.e., “the partial stability constant” and simple numerical addition can be used among the partial logarithm of the stability constant (PLSC), for explanation of the total stability constants. The structures of the rare earth—diethylenetriamine-N,N,N',N',N"-pentaacetic acid (DTPA) complexes in aqueous solution has been discussed from the point of PLSC.

Keywords: polyamine, polyacetic acid, stability constants, NTA, EDTA, DTPA

For the separations of rare earths by ion-exchange, mainly polyamine polyacetic acids, such as nitrilotriacetic acid (NTA) and ethylenediamine-N,N,N',N'-tetraacetic acid (EDTA) were used as the eluants. The DTPA complexes have attracted the attention as the effective paramagnetic compounds in MRI clinical studies.

The stability constants of the complexes of these amine polyacetic acids with rare earth ions have been extensively measured and compiled in several journals¹⁻⁶ and reference books⁷. These polyamine polyacetic acids have the same nitrilonitrogen group, a carboxy oxygen group, and -CH₂CH₂-moieties and only a difference in their number, namely, the analogous shape group.

The logarithm of the stability constant, $\lg K$, is related for the Gibbs energy change, ΔG , in the following manner

$$\Delta G = -2.303RT \lg K \quad (1)$$

The logarithm of the stability constant (LSC) is thermodynamically equivalent to the Gibbs energy change of the exchange reaction of water molecules bound to the central tripositive rare earth ion with coordinating groups of the ligands in the complex.

The Gibbs energy, ΔG , should be the sum of the Gibbs energy for each coordinating group. In other words, logarithm of the stability constant of a complex, $\lg K$, is considered to be the sum of the logarithm of the stability constant for the coordination of each coordinating group. We call the logarithm of the stability constant of the coordination for each coordinating group “the partial logarithm of stability constant (PLSC) in this article.

$$\Delta G = \sum \text{PLSC} \quad (2)$$

In the NTA complex, there are one amine nitrogen atom (N) and three acetate carboxyl groups (3 O). The logarithm of the stability constant of the NTA complexes is expressed as equation (3)

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