Statistical prediction for mixed uranyl complex formation in artificial seawater

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In a complexed electrolyte solution such as seawater the mixed complexes of uranyl can dominate over simple complexes in respect to the medium containing different types of ligands. One of the possible solution of this problem is based on theoretical modeling constants of mixed complexes.

DYRSSEN *et al.* (1968) model predicts the magnitude of mixed-ligand formation constants, $^{\beta}$a, b, from single-ligand type formation constants, $^{\beta}$N. Since seawater contains a variety of potent ligands, and mixed-ligand complexes are statistically favored relative to single-ligand type complexes, recent attempts to model trace-metal complexation in seawater have included calculations of stability constants of the following type:

$$\beta_{a,b} = \frac{(MX_aY_b)}{(M)(X)^a(Y)^b} = \frac{N!}{a!b!} (x\beta_N{}^{a} * y\beta_N{}^{b})^{1/N}$$

where:

$$N = a+b; \qquad x\beta_N = \frac{(MX_N)}{(M)\,(Y)^N} \qquad y\beta_N = \frac{(MY_N)}{(M)\,(Y)^N}$$

On the basis of this calculations the stability constants of the mixed uranyl-hydroxo-peroxo-carbonato species has been evaluated.

Including those equilibria and their corresponding stability constants into the developed model of seawater species distributions (DJOGIC *et al.*, 1986) the pH dependance of uranyl-species has been obtained.

The calculations show that a significant percentage (20 to 30%) of uranyl species should be in the form of a uranyl mixed complexes of ligands, such as -OH, $-CO_3$, especially in the pH range 6 to 8.

The calculations performed for the photic zones where the hydrogen peroxide is present as a potential ligand (DJOGIC and BRANICA, 1991), indicate the presence of the uranyl complexes with peroxide, as well.

REFERENCES

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