February 4th, 2025
11:00

Prof. Demetrio Milea
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BACKGROUND

Demetrio Milea is Professor of Analytical Chemistry at the CHIBIOFARAM Department of the University of Messina. His research activity is focused on the determination of thermodynamic formation parameters and chemical speciation modeling in real aqueous systems. His research activity is mainly carried out by Electrochemical, Spectroscopic, Spectrometric and Calorimetric techniques and specialistic software. He is co-author of more than 80 articles in ISI journals and 2 international book chapters (H-index = 28 with more than 1900 citations), and invited speaker at national and international conferences. He is Associate Editor and EB member of ISI journals in the field of analytical and environmental chemistry, editor of 2 international books and other serial publications. He was Action Chair of the COST Action CA18202 – NECTAR – Network for Equilibria and Chemical Thermodynamics Advanced Research and past-President of the International Group for the Thermodynamics of Complexes (ISMEC Group), and consultant of a multinational company for the design, modeling and chemical speciation of real systems and consumer products.

The paramount importance of chemical speciation studies in biology and environmental sciences. From theoretical to practical aspects, with emphasis on the case of rice fields in the ARSENIX project.

Abstract

Chemical Speciation (*CS*), as defined by IUPAC, is the "distribution of an element amongst defined chemical species in a system".

Since the chemical and physical properties of any elements of compounds are strictly related to the species in which they occur in particular conditions, *CS* studies are of paramount importance to evaluate their impact, activity and/or performances in real systems of environmental, biological and technological/industrial interest.

One of the most effective ways to perform *Speciation Analysis* is through computer modelling based on thermodynamic equilibrium data (mainly, but not only, stability constants). To this aim, reliable sets of formation constants are necessary to evaluate the network of the most relevant interactions between all components of the system under investigation.

Considering that several real systems (*e.g.*, seawater, estuarine and fresh waters, biological fluids, process and/or waste waters) are, from a chemical point of view, multielectrolyte aqueous solutions in which many elements and compounds are simultaneously present in a wide range of conditions, it is evident how *CS* studies of these systems represent a particularly challenging task.

Starting from the basic concepts regarding the chemical speciation of real aqueous systems, the talk will then focus on: i) the evaluation of the most critical aspects related to the experimental determination of thermodynamic parameters in multicomponent aqueous solutions; ii) their modelling as a function of chemical and physical variables like composition, ionic strength and temperature; iii) the use of computer tools and calculation approaches for data elaboration and speciation analysis; iv) examples and applications of speciation studies, with emphasis on the case of rice fields in the ARSENIX project.

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