“Speciation” Chemistry: Overdue for a Resurgence

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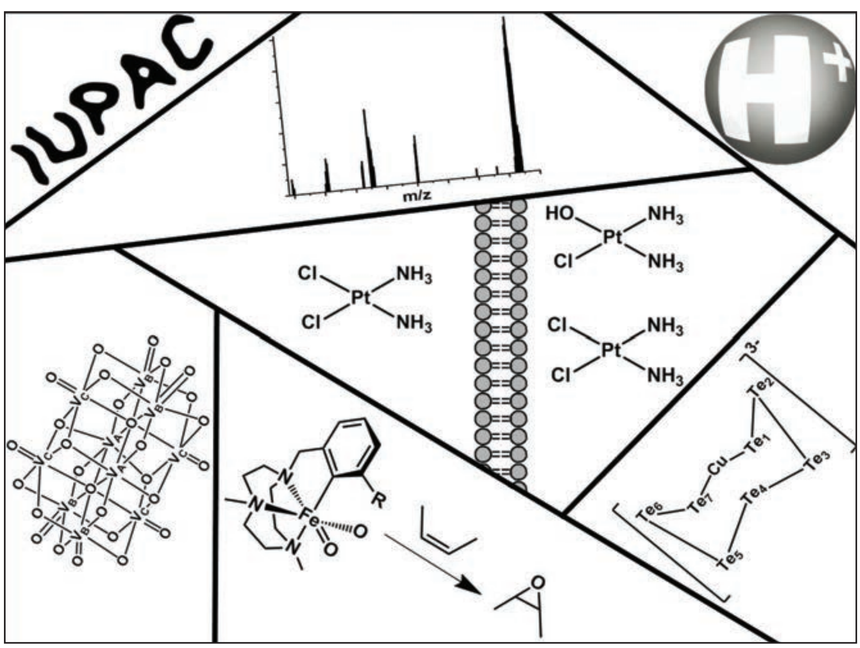
The idiom, “the devil is in the details” refers to situations in which some easily-overlooked detail is critical to success. This idiom in a sense embraces some concepts of certain areas of speciation chemistry in which details are so critical for the proper description of a system and depend on a complex interplay of the composition and state of the system. Undoubtedly, specific conditions, such as pH, temperature, and system components, are instrumental to describing so many areas of speciation in chemistry. Unfortunately, in the past traditional research in the speciation field has not received the same limelight that other aspects of chemistry do, despite its importance to our fundamental understanding of chemistry as a whole. Regardless, an increasing number of contributions in speciation chemistry have emerged, although these may not include speciation chemistry as it was originally defined. One recent highlight is the special issue on speciation chemistry just published as a volume of *Coordination Chemistry Reviews* [1,2]. This issue compiles papers that illustrate some of the areas in speciation chemistry and document how the field has evolved [2,3], its interplay with IUPAC [4], and specific examples of how traditional speciation chemistry has changed [5-10].

Speciation chemistry, as originally defined by classical solution chemists [11], has been significantly expanded. Although the terms “chemical species” (the specific form of chemical elements or an element defined by its isotopic composition, electronic or oxidation state, and/or complex or molecular structure) and “speciation analysis” (analytically identifying and/or measuring the quantities of one or more individual chemical species in a sample) are readily used [11] by chemists. This definition, when expanded, encompasses much more that is particularly relevant for modern society and chemists. Several examples of modern approaches to speciation chemistry exist and are actively in use. For example, a speciation chemist with an analytical focus may be more concerned with methods and characterization that may involve the isolation or simply the identification of different forms [12,13]. Other advances in areas of speciation chemistry have led to the development of new methods. For example, the availability of various types of mass spectroscopy allows for the characterization of many new systems, as well as other advances in areas of analytical chemistry.

Inorganic and organic chemists would include structure as an essential component to speciation. In organic chemistry, chirality and conformations resulting in shapes are often critical definitions that reach into all the biological areas of sciences. Similarly, in inorganic chemistry, particularly in coordination chemistry, the formation of complexes is so intrinsically linked to structure and shape that the composition of a system only defines part of the system [3-10].

Given the changing times and the importance of the “devil in the details”, many more chemists find themselves involved in work that, in a broad sense, can be characterized as speciation chemistry. After all, providing the specific conditions that make the



Images representing contributions to the volume on Speciation Chemistry reported by Coord. Chem. Rev. *2017, volume 352, The “Pourbaix diagram representing speciation chemistry 2017” was created by Cameron Van Cleave for the volume cover.*

chemistry 'work' requires attention to detail. It is perhaps no surprise, then, that speciation is finally getting some long overdue credit and attention. Speciation chemistry is, and remains, a pillar of solution chemistry, but it is only slowly being recognized that nanochemistry and solid state chemistries are also intrinsically dependent on the detailed chemistries—that is, the nature of the species that exist, the conditions in which they exist, and their reactivity. These are exciting times, and the applications of speciation chemistry seem endless. It is hoped that this recognition will bring to the table a newfound approach that will assist modern practitioners of speciation chemistry in demystifying their chemistry and providing a platform for progress and discovery. Presentations on the topic of speciation in the modern sense are sought for the International Coordination Chemistry Conference in Sendai, Japan [13].

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IUPAC Silver book—corrigendum

In April 2017, *Chemistry International* announced the release of the second edition of the so-called IUPAC Silver book, *i.e.* the "Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences" [1]. The authors of the Silver Book have since shared a change to Section 6.10.5. The description of how the combined standard measurement uncertainty is obtained has been rephrased in order to conform with the International vocabulary of metrology (JCGM 200:2012 International vocabulary of metrology—basic and general concepts and associated terms (VIM), BIPM, Sèvres. www.bipm.org/vim).

Section 6.10.5 now reads:

> Each component of measurement uncertainty estimated by Type A or B evaluation can be characterized by a variance, u^2, that may be calculated from the distribution of values with repeated measurements (Type A) or assessed by using available knowledge (Type B). The positive square root of such a variance is called **standard measurement uncertainty,** u. Standard measurement uncertainty values may be combined by the law of propagation of uncertainty [JCGM 100: 2008, section 5]: the result is called the **combined standard measurement uncertainty**, u_c [ref. 20, concept 2.31]. Such a quantity has the same dimension as the quantity being measured and is expressed in the same unit.

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