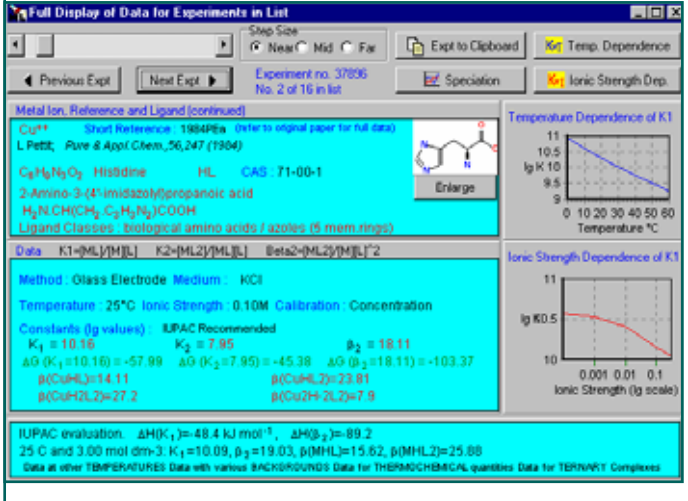
The following review introduces a new series of articles on "Tools of the Trade," which will provide a forum for views and discussion on one of the Union's goals: "IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion."

The series, which will run through 2006–2007, was initiated by Kip Powell, past president of the IUPAC Analytical Chemistry Division (Division V). It will allow for a presentation of key outputs from IUPAC projects and will cover all fields of chemistry. As well as informing readers, it is hoped that the series will renew awareness of the valuable contributions IUPAC continues to make in facilitating the advancement of research in the chemical sciences. If you wish to contribute to this series, please contact <kip.powell@canterbury.ac.nz>.

The IUPAC Stability Constants Database

by Leslie D. Pettit

Metal-ligand stability constants (SC) are of vast importance to all scientists (not just chemists) working quantitatively in solution. IUPAC has been actively involved in the compilation of literature values of such constants for over half a century. The project was first considered in 1951 and the first compilation was published in 1957 under the auspices of IUPAC. This was followed by further volumes in 1964, 1971, and 1983. The editors of these volumes, which included data to about 1973, included most of the major pioneers in the field: G. Schwarzenbach (Switzerland), L.G. Sillen (Sweden), G. Anderegg (Switzerland), J. Bjerrum (Denmark), A. Martell (USA), H. Irving (UK), E. Högfeldt (Sweden), and D. Perrin (Australia).



Background to SC-Database

A mainframe computer-based system was proposed in 1979 and trialled in Stockholm. A PC-based system was proposed in 1989 and a FORTRAN-based version was first demonstrated by Academic Software in 1991. Data from the book-based compilations were added over the following years using specially prepared software. Software was subsequently rewritten for 16-bit Windows operating systems, followed by fully object-orientated versions for 32-bit Windows using fast, indexed searching techniques. The graphical interface was further improved by including structures for ligands in mol-file format and routines for substructure searching—essential for distinguishing similar ligands. Routines for comparing the stabilities of complexes with specified metals and for faster journal and reference searching were also added. Interactive graphical speciation software was included.

Overview of SC-Database

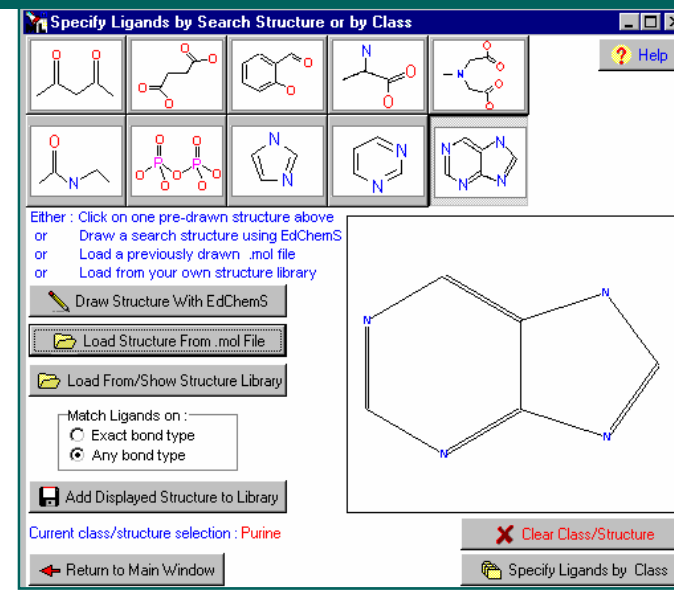
The SC-Database is a compilation of all significant metal-ligand complex stability constants published in the scientific literature. The database, which is regularly updated and maintained, currently includes data from 1887 to 2004/5 on over 9200 ligands from over 22500 references in 108000 records. It holds all data previously published in the book volumes (about 35 percent of the total) and completely supersedes them. Data held includes ligand details (full and short name, empirical formula, CAS-registry number, and structure) metal ion details, full literature reference, many experimental details (method used, temperature, and ionic background), published values of stability constants and protonation constants) and other data as available (e.g., solubility product, ΔH_r values). On entry, the constants are not critically evaluated, but where they have been evaluated in parallel projects by the Analytical Chemistry Division (V), the IUPAC-rec-

ommended values are also included.

Searching is designed to be fast and flexible. The database may be searched on any fragment of a ligand name (not necessarily the start), author, or journal, on experimental conditions, for a range of temperatures, range of numerical values of a constant, or any fragment of a descriptive comment. It is also possible to enter a ligand substructure fragment (in mol-file format) and to search the entire ligand database for ligands containing this fragment. The structure fragment may be prepared by any major structure-drawing program, or by the program EdChemS which is provided with SC-Database.

Peripheral Programs

The speciation program is a powerful attribute. It has many applications, such as calculation of species distribution curves, calculation of pM or pL values as a function of solution pH and stoichiometry, and the determination of solution stoichiometry required for metal ion buffers. It can handle a mixture of up to 11 reactants and 30 constants (including solubility products). Data may also be used in programs for ionic strength and temperature corrections prepared as part of the IUPAC project on ionic strength corrections. These are supplied with SC-Database and are also available separately from <www.iupac.org/projects/2000/2000-003-1-500.html> or from <www.acadsoft.co.uk/aq_solutions.htm>. Output (text and graphical) can be directed to disk, to printer, or to the clipboard in a selection of formats.



Database Maintenance and Availability

The SC-Database suite of programs has been developed and is maintained by Academic Software. Data collection and compilation is in close collaboration with the IUPAC Analytical Chemistry Division. SC-Database is currently managed and distributed by Academic Software (Leslie and Gwyn Pettit) for IUPAC. An order form, a demonstration database, and additional details can be accessed via <www.acadsoft.co.uk> or <www.iupac.org/publications/scdb>.

Beyond Classical Chemistry

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we'll be extinct in a generation."[27] However, other chemists instead emphasize the need for classical chemical knowledge in the broader and even more heterogeneous field of MS: "As the borders between scientific disciplines blur (a process that will only continue), fundamental chemistry skills such as synthesis and analysis will be crucial for the interdisciplinary subjects that emerge."[28]

With increasing interaction between the classical sciences and also between science and society, the meta-molecular fields discussed in this article are needed to give perspective and guidance to and about the practitioners and teachers of the molecular sciences. It is time to redefine ourselves as (meta) molecularists.

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27. Birkett, D. (2001) "Yuletide, Chemical Warfare, and Essential Micronutrients" *Chemical Innovation* 31(12):IBC.
28. Editorial (2001) "A Discipline Buried by Success" *Nature* 411:399.