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).

The IUPAC Stability Constants Database

by Leslie D. Pettit

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, $\Delta H_r$ 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

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 metamolecular 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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www.fpi.lu.se/en/sjoestroem