chain; trace elements in food (occurrence and function); interaction of trace elements with other compounds (toxicological and nutritional aspects); trace element speciation in food and its implications for human health; advances in methods for analyzing trace elements in food matrices; and quality assurance and reference materials for the analysis of trace elements in food. Of particular note among the presentations were those that provided an insight into areas of future development, for example, tackling the question of how far we are today and where we are going with international legislation on trace elements as contaminants in food. The extent to which the uptake of Cu, Se, Zn, Ni, Mo, and Cr fulfils dietary needs was assessed with respect to the Austrian diet. The use of stable isotopes to determine bioavailability of trace elements was assessed, as was speciation of trace elements in terms of what we presently know and what we need to know for the future. Finally, the important area of measurement in food was discussed from a metrology viewpoint, as was the question of traceability in food measurements.

The proceedings of the symposium, edited by Prof. Szteke and including the oral contributions, will be published before the end of 2001 as a Special Issue of *Food Additives and Contaminants*.

The Commission on Food (VI.5) will be disbanded by the time of the next symposium, owing to the upcoming restructuring of IUPAC. It is hoped, however, that the success of this first symposium will lead to a second symposium, which probably will be hosted by the Institute for Reference Materials and Measurements (IRMM) in Geel, Belgium in 2003.

Prof. John Gilbert
Chairman, IUPAC Commission on Food (VI.5)
Ministry of Agriculture, Fisheries, and Food
Central Science Laboratory
Sand Hutton, York, England, UK

New Projects

Visit http://www.iupac.org/projects/ for complete information and further links.

IUPAC Chemical Identifier (IChI)

IUPAC has approved a project to establish a unique label, the IUPAC Chemical Identifier (IChI), as a nonproprietary identifier for chemical substances that could be used in printed and electronic data sources, thus enabling easier linking of diverse data and information compilations.

IChI will not require the establishment of a registry system. Unlike the CAS Registry System, it will not depend on the existence of a database of unique substance records to establish the next number for any new chemical substance being assigned an IChI. It will use a yet-to-be-defined set of IUPAC structure conventions, and rules for normalization and canonicalization of the structure representation to establish the unique label. It will thereby enable an automatic conversion of a graphical representation of a chemical substance into the unique IChI label, which can be performed anywhere in the world and which could be built into desktop chemical structure drawing packages (such as ChemDraw, ISIS/Draw, etc.) and online chemical structure drawing applets (such as ACD/Draw).

IUPAC would define the process flow leading from input of structural information to the creation of the Identifier in three steps: definition of chemical structure input requirements, algorithms for generating a unique set of atom labels (canonicalization), and algorithms for conversion of these labels into the Identifier (serialization). Structure input and conversion to the structural format required by the IChI generator would be carried out with vendor-developed software.

The process would be reversible, so that the Identifier output could be used to regenerate structural input information. The Identifier would thus serve as the computer equivalent of the IUPAC name for a molecule. This arrangement would facilitate searching the Internet and labeling information in electronic documents with the name of the chemical substance in question.

A prototype algorithm with limited applicability is expected to be available for testing toward the end of 2001.

Comments from the chemistry community are welcome and should be addressed to the project coordinator, Dr. Alan McNaught, General Manager, Production Division, RSC Publishing, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, England, UK, Tel.: +44 1223 432119, Fax: +44 1223 420247; E-mail: adm@rsc.org.

See http://www.iupac.org/projects/2000/2000-025-1-050.html for project description and update.

Immunochemistry of Metal Sensitization

A number of metals are immunological sensitizers in humans. Examples include occupational exposures to Ni, Co, and Cr; inhalation of Pt compounds and the possibility of sensitization to chloroplatinic catalysts in silicone implants; beryllium-related lung disease; and exposure to components of alloys used in joint replacements and skeletal stabilization. In general, activation of the immune system occurs when the metal ion (hap-

ten) binds to an endogenous protein carrier, altering its structure and causing it to become antigenic. T-cells may recognize metal-modified peptides or the T-cell's MHC class II-peptide complex may itself be modified by a metal ion. The nature of the metal hapten-carrier complex has not been systematically reviewed for metals that are important occupational or iatrogenic immunosensitizers. New immunological methods are being developed for clinical evaluation of immune sensitization by a number of occupationally and iatrogenically important metals.

IUPAC has approved a two-year project to evaluate and systematize the application of these methods, and to produce a critical examination of the molecular structural foundations of the sensitizing response.

Comments from the chemistry community are welcome and should be addressed to the task group chairman, Prof. Douglas M. Templeton, Department of Lab Medicine and Pathobiology, University of Toronto, Medical Sciences Building, Room 6302, 1 Kings College Circle, Toronto, Ontario M5S 1A8, Canada; Tel.: +1 416 978 3972; Fax: +1 416 978 5959; E-mail: doug.templeton@utoronto.ca.

See http://www.iupac.org/projects/1999/1999-047-1-700.html for project description and update.

Critically Evaluated Termination Rate Coefficients for Free-Radical Polymerization. 1. Current Status, Evaluation of Experimental Methods, Data for Styrene and Methyl Methacrylate

Free-radical polymerization (FRP) has always been a scientifically and commercially important field. This importance is set to increase even further owing to recent advances such as the development of "controlled radical polymerization". Hence, it is of great benefit for both science and industry to be able to model the kinetics of FRP systems. Such modeling is dependent on the availability of reliable values of rate coefficients, but attaining such values is not as straightforward as one might suppose. An IUPAC Working Party on Modeling of Polymerization Kinetics and Processes has outlined the reasons for this situation [1,2] and has begun to rectify it with regard to propagation rate coefficients [3–5]. Now this process will be started for termination rate coefficients, k_t.

This collaborative project, supported by IUPAC's Macromolecular Division (IV), brings together experts in the field in order to fulfill the following goals:

- To make workers aware of the subtleties involved in studying and describing the termination reaction;
- To carry out an evaluation of methods for determining k_t, arriving at agreement regarding the strengths and weaknesses of each method; and
- To come up with critically evaluated k_t values for the initial stages of bulk polymerization of styrene and methyl methacrylate, two otherwise well-characterized systems.

This project is being chaired by Dr. Greg Russell, who may be contacted at: Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch, New Zealand; Tel.: +64 3 364 2458; Fax: +64 3 364 2110; E-mail g.russell@chem.canterbury.ac.nz. Comments and suggestions will be welcomed. See http://www.iupac.org/projects/2000/2000-028-1-400.html for project description and update.

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Metabolism Terms

IUPAC has approved a new project to list and define terms pertinent to the area of drug metabolism. The resulting list will be disseminated to the scientific community via publication in relevant journals. This process will help achieve a common definition base across the various publications and databases pertaining to the drug metabolism field, particularly with regard to the latter's impact upon chemical structure.

Comments from the medicinal chemistry and drug metabolism communities are welcome and should be addressed to the project chairperson, Prof. Paul Erhardt, Center for Drug Design and Development, The University of Toledo College of Pharmacy, Toledo, Ohio 43606-3390, USA; Tel: +1 419 530 2167; Fax: +1 419 530 1994; E-mail: perhard@utnet.utoledo.edu.

See http://www.iupac.org/projects/2000/2000-009-1-700.html for project description and update.