Global Availability of Information on Agrochemicals

A tremendous amount of information related to the chemistry of agrochemicals has been generated, which resides not only in the open literature but also in various government and industry files. This information includes reports and recommended approaches developed by IUPAC projects on agrochemicals during the past 20 years. Also included are unpublished reports and technical summaries of information from various advisory bodies, regulatory agencies, and individual agrochemical companies.

However, there is a lack of coordination to make this information widely available to interested regulators and research scientists on a worldwide basis. As a result, decisions at a local level may be made or new research programs initiated without taking into account available information. Thus, the Food And Agriculture Organization of the United Nations and the International Atomic Energy Agency (FAO/IAEA) has initiated a project entitled INFOCRIS (International Food Contaminant and Residue Information System), which will utilize the Internet and CD-ROMs, to make agrochemical information more widely available to scientists in developing countries.

However, the FAO/IAEA currently lacks the capability to populate the data matrix that has been created regarding information on agrochemical properties. Other organizations (e.g., Oregon State University, U.S. Environmental Protection Agency, Pesticide Action Network [PAN]) are independently developing information systems on the Internet. With such a multitude of sites offering information on agrochemicals, there is a need to establish an authoritative site which can ensure the involvement of all information owners in the process.

IUPAC offers the opportunity for an unbiased and authoritative effort based on the collaboration of government, academic, and industry scientists. In addition, IUPAC reports and recommendations related to agrochemicals are poorly known and underutilized, and wider circulation on the Internet will increase the profile and influence of the Union. Finally, access to information on the most recently introduced pesticides tends to be difficult to obtain, and involvement of industry in the IUPAC project will provide access to a major, untapped source of information.

The outcome of this project will increase the global availability of information on the chemistry of agrochemicals, including methods for testing and evaluation, summaries of properties for individual pesticides, and regulatory standards for pesticides.

Meetings and telephone conferences have been held with FAO/IAEA and the INFOCRIS project manager in order to begin cooperation. Based on these communications, it was agreed that some of the tables in the INFOCRIS system should be modified so that they were more closely aligned with the criteria laid down in the project description. These changes were adopted by FAO/IAEA and, thanks to their support, have now been put in place. Consequently, a revised version of INFOCRIS will be available shortly.

Additionally, a meeting was held with members of the IUPAC project titled “A Critical Compendium of Pesticide Physical Chemistry Data” (# 2003-011-3-600) so that information from this project could be utilized. As a result of these meetings, an initial list of 60 agrochemicals has been chosen for inclusion in the INFOCRIS/IUPAC project. Again, thanks to the support of FAO/IAEA, the majority of profiles for these agrochemicals are now being prepared.

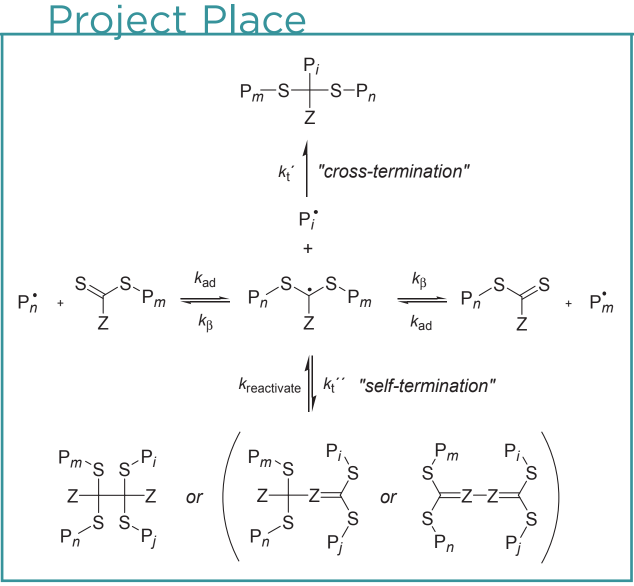
A draft Web page has been proposed and submitted to members of the task group and discussed at a recent meeting of the Advisory Committee on Crop Protection Chemistry in Costa Rica (see Conference Call, p. 34). At this meeting a timetable was agreed upon for the project. The proposed launch for the IUPAC Web page on “Information on Agrochemicals” is the IUPAC Pesticide Congress, which will be held in Kobe, Japan, in August 2006 (See Where 2B & Y, p. 38).

For more information and comments, contact the Task Group Chairman John Unsworth <johnlydiaunsworth@compuserve.com>.

www.iupac.org/projects/2001/2001-022-1-600.html

Towards a Holistic Mechanistic Model for Reversible Addition Fragmentation Chain Transfer (RAFT) Polymerizations

The goals of this project, which emerged from activities of the IUPAC Subcommittee on Modeling of Polymerization Kinetics and Processes, are to develop a detailed understanding of the mechanism of the reversible addition fragmentation chain transfer (RAFT) polymerization and determine the correspon-



The basic RAFT reaction scheme (middle), which induces an equilibrium between propagating radicals, $P_n^\bullet$ and $P_m^\bullet$, possibly needs to be extended by reversible and/or irreversible termination reactions of the intermediate radical (center) with either another propagating radical, $P_i^\bullet$, (upper part) or with itself (lower part) to correctly describe the kinetics of the process.

ding kinetic coefficients. Whereas reliable information about propagation and—at least to some extent—termination rate coefficients for the modeling of radical polymerization processes has been made available by a number of IUPAC projects, the situation is less satisfying with regard to the mechanism and kinetics governing the RAFT process. Although it is widely used for the generation of both complex and well-defined polymeric materials—especially those employing dithioester compounds as the mediating agents—a complete understanding of the fundamental RAFT reaction scheme, which induces the equilibrium between dormant and active radical species, has not yet emerged. A deep understanding of the RAFT process, however, is mandatory to establish structure/rate correlations for a specific RAFT agent, which is essential for rational RAFT agent design delivering novel mediating compounds.

A wide variety of advanced techniques have been applied in recent years to elucidate the mechanism of RAFT polymerization and to arrive at rate coefficients describing the RAFT equilibrium reactions. It has been demonstrated that the choice of the reaction scheme operative in the RAFT process shows a significant influence on the rate coefficients obtained by the experimental methods presently available. In addition, some of the disagreement in the literature may stem from the fact that vastly differing reaction conditions have been employed in the individual studies.

This project aims to improve the currently obscure situation by assembling a team with expertise in free radical polymerization kinetics, mechanism and synthesis, as well as quantum mechanics. The evidence gathered by different scientific groups and experimental results for various RAFT systems will be collated and critically evaluated. The current situation, including common agreement and outstanding inconsistencies, will be assessed in detail. Subsequently, recommendations will be given on how to rationally perform and present future kinetic RAFT experiments to guarantee comparability.

The project aims to formulate a holistic mechanistic model for dithiobenzoate-based RAFT processes of common monomers and to critically evaluate kinetic parameters for dithiobenzoate mediated polymerizations of styrenics, methacrylates, and acrylates. Dithiobenzoates are important RAFT agents for the generation of well-defined polymers, and reasonable kinetic parameters for these mediating agents are of priority to the scientific community.

For more information and comments, contact the Task Group Chairman Philipp Vana <pvana@uni-goettingen.de>.

www.iupac.org/projects/2004/2004-040-1-400.html

Guidelines for Potentiometric Measurements in Suspensions

This project aims to unambiguously define and interpret the suspension effect (SE) on the basis of recent experiments. It will take into account the enormous amount of theoretical and experimental work accomplished in 75 years since the term was first introduced—a period in which no consensus was achieved. On the basis of the recommended definition and interpretation, the significance of potentiometric measurements in suspensions performed in different ways will be explained.

The SE is defined as the difference of the galvanic cell voltage measured with the electrodes (i) in the equilibrium solution of the suspension and (ii) in its sediment. It will be argued that the SE should be regarded as the sum of two effects that occur when the electrodes are immersed in a suspension. These are (i) the transition of the indicator electrode from a reversible potential to an irreversible mixed potential, and (ii) a systematic error of