Additions and Corrections

Synthesis, Structure, and Reaction of the First Thermally Stable *cis*-(Silyl)(stannyl)palladium(II) Complex [*J. Am. Chem. Soc.* **1995**, *117*, 6408−6409]. MASAHIRO MURAKAMI,* TAKASHI YOSHIDA, SHINICHI KAWANAMI, AND YOSHIHIKO ITO*

Page 6409: We acknowledge the following precedent papers proposing the same mechanism involving a zwitterionic carbene complex for the formation of trans-adducts in the palladium-catalyzed 1,2-addition reaction to an alkyne: Zargarian, D.; Alper, H. *Organometallics* **1993**, *12*, 712−724. Chatani, N.; Morimoto, T.; Muto, T.; Murai, S. *J. Organomet. Chem.* **1994**, *473*, 335−342.

JA9550283

Computer Software Reviews

Scientist for Windows. Version 2.0.. MicroMath Scientific Software: P.O. Box 21550, Salt Lake City, Utah 84121; (801) 943-0290, (801) 943-0299 FAX. List Price $395.00; educational discounted price $295.00.

Scientist Version 2.0 is an impressive addition to any scientist's software collection. This scientific analysis and data fitting program is written for DOS-based computers running Microsoft Windows 3.1 and higher. It will run on a 386 or higher computer with at least 4 MB of RAM and ~5 MB available hard disk space. As with most Windows programs, having more memory and a faster processor can only help the performance of Scientist. Scientist comes on two 1.44 MB ($3^1/_2$ in.) disks and also includes an equation editor similar to that found in Microsoft Word. The license allows the user to make backup copies with the provision that it not be used concurrently on more than one computer.

The standard Windows interface and simple menu options minimize the learning curve. To handle any complex model, the program breaks it down into small steps. The first step is model entry. The user can enter equations defining their system of choice with independent and dependent variables and parameters that are to be fitted. Equations that are entered can have variable names that are easily understood such as PKHA for the pK_a of an acid. The model window also contains user-definable equations and makes use of several defined equations such as a derivative and integration function. These and other predefined functions add to Scientist's ability to model almost any given situation. If experimental data are available the user can also call up minimization routines for parameters or plot the data and select the best fit. Data can be generated by entering parameters and a range for the independent variable(s). From these data, plots can be made and statistical output can be generated.

Also included in the package is a Worksheet window. In this window simple math like addition or multiplication can be performed by just entering 2*3 followed by a ⟨Ctrl+Enter⟩. The user is not limited to simple math. A host of trigonometric, statistical, and bit-level functions are included to aid in the evaluation of complex functions. The worksheet also supports units. Units can be added to values and can be converted to other units. All SI units and other more obscure units, along with many useful constants, eliminate the need to perform dimensional analysis and permit the user to focus on the problem itself rather than how to calculate the answer. As with most Windows programs, the text in the worksheet window can be cut and pasted into any word processing document. The equation editor is a nice addition to the Scientist software package but those users who have Microsoft Word will find it unnecessary.

A 500+ page manual is included which enables the user to quickly learn the basics of the software as well as explore the full power that is included. The manual is very informative and includes many examples with helpful screen shots. Each aspect of the program has a chapter devoted to it that completely explains its usage. An "Example Calculations" chapter provides specific examples ranging from acid/base chemistry and kinetics to physics and electronics. These examples show how easy it is to solve the given problem with a simple understanding of the equations that define the problem. Specifically, an example on chemical equilibrium is very informative. In this example, a polyprotic acid is studied to show the buffer capacity as a function of pH. Every chapter has specific examples which focus solely on the topic at hand. Besides useful examples, Scientist also has a wide breadth of topics. Focusing on the numerical methods, Scientist includes support for methods such as Euler's method, fourth-order Runge−Kutta, error controlled Runge−Kutta, and Bulirsch−Stoer's method.

The examples show that Scientist would be a useful tool in an academic setting, but they also easily suggest the flexibility and power available for utilization in an applications or research environment. The one unfortunate aspect of the software is the use of multiple files for a given problem. A separate file is generated for the model definition, the parameters, the data, and every plot. A possible enhancement would be to incorporate the ability to save a project that would include all of the previously mentioned elements.

In short, Scientist provides an excellent mathematical package, providing a wide range of modeling, data fitting, and plotting capabilities. The manual, in combination with help screens, presents a relatively shallow learning curve for "testing the waters". Once initiated, the manual then serves as a useful resource to maximize the utility of this package.

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JA9558610

Book Reviews

Environmental Epidemiology: Effects of Environmental Chemicals on Human Health. Advances in Chemistry Series Volume 241. Edited by W. M. Draper (California Department of Health Services). American Chemical Society: Washington, DC. 1994. xii + 266 pp. $79.97 (hardcover), $49.95 (paper). ISBN 0-8412-2517-6 (hardcover), 0-8412-2933-3 (paper).

The comprehensive toxicity information needed to conduct an adequate risk assessment exists for relatively few of the over 60 000 commercial chemical entities to which humans may be exposed; this situation exacerbates public fear and chemophobia. Environmental risk assessment using safety data generated with rodent bioassays will encounter problems of extrapolation across species and to the lower

doses to which humans are exposed. These problems combined with ethical constraints on human testing mean that, for most environmental chemicals, epidemiological studies, which search for correlations between inadvertant exposure and adverse biological effects, afford the only means for determining such effects in humans. Exposure assessment is the weak point of environmental epidemiology; greater rigor would be injected into environmental epidemiological studies if better measures of the doses received by members of the study population became available.

This volume is intended to introduce the concepts of environmental epidemiology and risk assessment to the chemist; an important element of this is to explain how epidemiology is very different from the highly controlled, reductionist type of science practiced im the chemical laboratory. With this knowledge the chemist can go about developing biomarkers of exposure to environmental chemicals that might properly meet the exposure assessment needs of the epidemiologist. Chapter 1 of this volume sets the tone by underlining the need for human-based epidemiological evidence, through illustrations of how animal-based toxicity information can lead to incorrect conclusions about the magnitude of risk to humans. Chapters 2−4 are brief overviews of the different types of epidemiological investigations, their design, interpretation, and limitations. Chapters 5−8 describe principles and methods of general, reproductive, developmental, and genetic toxicology and the risk assessment framework that utilizes laboratory test and human epidemiological data. Chapter 7 and 8 have a strong focus on short-term in vitro tests. The reason for including such a focus in the volume is unclear unless the reader knows that the lack of adequate safety information for so many compounds and a desire to use fewer animals in testing stimulated the development of rapid and inexpensive in vitro methods capable of detecting significant hazards; however, while useful within certain limitations, these tests suffer from an even greater extrapolation to human experience than is seen with animal studies. This reiterates the importance of good human epidemiological information to risk assessment.

Most of the remaining chapters deal with issues of assessing exposure and biological outcome that call for input from chemists and biochemists. Chapters 9 and 10 focus on the development and use of biomarkers of internal dose and biologically effective dose, those portions of the external dose/exposure that actually enter the body and cause biological responses, respectively. Chapters 10−15 are case studies on 1,3-butadiene, acrylonitrile, cadmium, malathion, and metam sodium which illustrate the development of specific internal biomarkers of exposure and biological response in humans and their use in determining internal or biologically effective doses to correlate with biological outcome or calculating what levels of external exposure give rise to what internal or biologically effective doses. The barriers to obtaining information relevant to epidemiological studies, described in Chapter 16, should be of concern to all.

The final chapter draws together the central themes described at the beginning of this review; however, it is not the only place this occurs. The editor and chapter authors should be commended for developing a set of cohesive themes and coordinating the separately authored chapters so the reader understands how they fit into the thematic framework; Chapter 6 is particularly good in this regard. The volume is comprehensive on the subject of the value of biomarkers of exposure to epidemiology. Some additional uses that are not emphasized are worth noting; biomarkers of exposure can also be used to detect susceptible and resistant individuals in a population, measure the efficacy of interventions designed to mitigate the adverse effects of exposure, and help elucidate mechanisms of toxicity.

Initially, this reviewer was concerned by the long lag time that seems to be inevitable when volumes derived from conferences, such as this volume, are brought to press; most of the revised chapter manuscripts were submitted in 1992−93. However, since the volume is a primer intended to introduce the chemist to the nature of epidemiological studies and illustrate how chemistry can contribute to these studies, the lag is not a problem.

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JA945160N

Engineering Risk Analysis of Water Pollution, Probabilities and Fuzzy Sets. Edited by Jacques G. Ganoulis (Aristotle University of Thessaloniki). VCH: Weinheim, Germany. 1994. xi + 306 pp. $80.00. ISBN 3-527-30050-3.

Noting that "risk and reliability analysis is a relatively new subject in water resources and environmental engineering", the author offers this book as a text "for understanding and using this powerful new tool." The book is aimed at graduate students, engineers, hydrologists, and other professionals working on environmental water quality issues. The book is divided into six chapters, the first of which provides a broad introduction to water quality, water pollution, and water management as well as perspective on the need for risk and reliability assessment in these areas.

Chapter 2, which is entitled Risk Identification, includes some essential (and some nonessential) concepts of probability theory and fuzzy sets. In introducing risk assessment, the author paraphrases the three key questions: What could go wrong? How likely is it? and What would be the consequences? The emphasis throughout the text, however, is on estimating risk as the probability (or frequency) of a load exceeding a resistance, usually a pollutant concentration exceeding a water quality standard. Risk assessment activities dealing with the systematic delineation of scenarios that could potentially lead to exceedance and with the economic, health, and environmental consequences of exceedance are not emphasized. Unfortunately, this probably reflects the state of the art in environmental risk assessment.

In Chapter 3, Risk Quantification, the author distinguishes two situations. The first occurs when large quantities of data permit distributions on loads and resistances to be derived on the basis of classical statistics. The second situation occurs when when data are more sparse. In this case, the author advocates uncertainty analysis by the propagation of fuzzy numbers through models. To do this one must represent each uncertain model input as a fuzzy number and assign a credibility level to each value in a range. The Bayesian alternative of propagating prior/posterior probability distributions, which is by far the most common approach to uncertainty analysis applied in formal risk assessments, is not covered.

Chapter 4 discusses potential pollution threats in coastal water, river water, and ground water and provides a good survey of phenomenological modeling approaches including random walk models. Chapter 5, which is entitled Risk Management, presents a fairly standard treatment of decision analysis with examples related to water pollution. Chapter 6 provides an interesting summary of research performed by the author and his associates on river water, ground water, and coastal water quality and pollution issues.

The book contains far too many grammatical errors. Most of these appear to result from poor translation to English. With the exception of a discussion that ends prematurely at the bottom of page 27, these errors are more an irritant than a serious impediment to the reader. The examples that are presented in the book are, for the most part, helpful and relevant. Some, however, like the analysis of the impact of global warming on coastal water quality presented in Chapter 6, are grossly oversimplified. No student exercises or problems are included.

In spite of its deficiencies, the book deserves consideration by risk analysts interested in water pollution and by professionals dealing with water management.

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Progress in Inorganic Chemistry. Volume 42. Edited by Kenneth D. Karlin (Johns Hopkins University). Wiley & Sons: New York. 1994. 606 pp. $125.00. ISBN 0-471-04693-0.

This is the 42nd volume in one of the premier series of specialized reviews in inorganic chemistry. It is consistent with the high caliber of reviews of previous volumes. The contents include five articles: Slow Proton-Transfer Reactions in Organometallic and Bioinorganic Chemistry (Kramarz and Norton), Higher Oligopyridines as a Structural Motif in Metallosupramolecular Chemistry (Constable), Ternary Transition Metal Sulfides (Eichhorn), Organoimido Complexes of the Transition Metals (Wigley), and Palladium Complex Catalyzed Oxidation Reactions (Heumann, Jens, and Réglier). The reviews are comprehensive. The references are exhaustive and up to date. The senior authors are leaders in each of the areas. Their articles are intelligently organized and well-written and are easily read.

This is a book that every research library will reflexively order.

Edwin H. Abbott, *Montana State University*

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