THE COBLENTZ SOCIETY

NEWSLETTER

No. 100

A Society for Applied Spectroscopy Affiliate
Editor: T. Hirschfeld

July/August 1984

PRESIDENT'S MESSAGE

In the past year the Coblentz Society has made much progress, but we have a long way to go. One important goal that has been accomplished is much better communications with the membership. Through Jim de-Haseth and Kathy Kalasinsky, membership and publicity chairmen, respectively, we have enrolled more members, have had more mailings to members, and have greatly improved our membership database. The Coblentz Society has had a very active role in six spectroscopic meetings where we have set up booths, sold T-shirts and memberships and sponsored students and forums for scientific exchange via wine and cheese gatherings, etc. We are becoming much more active in the West Coast having been involved in the Pacific Coast Conference and the Western Spectroscopy Association Conference at Asilomar. Soon we plan to be much more international in scope. Although our international membership is low, we often have many Coblentz Society Award nominations and recipients from countries outside of the United States. Therefore in the future months I hope to set up an international committee for fostering our interests beyond the 50 states.

In addition to membership, we are very involved in technical matters. We have several active committees, from ones in digitization, spectral evaluation, etc., to ones in long range planning. Due to the foresight of our immediate past President, Bill Harris, we now have an endowment fund to add stability to our financial status, and have a much more pragmatic arrangement with our investment programs. However, the real progress is yet to be seen. The ball is rolling and gaining momentum. Everyone is to be congratulated for pulling together. For that I am personally very grateful.

Finally, I'd like to extend my warmest congratulations to Larry Nafie and Rod McDowell for being selected as new members of the Board. Their abilities will add another dimension to the Society. Thanks are also due to Tom Malloy and Hugh Diem for their years of dedicated service to our Society.

ALBERT B. HARVEY
The Coblentz Society

T-SHIRTS!

The Coblentz Society is selling T-shirts. These were a smash hit at several conferences last summer and are sold out. However, we now have a new, even "jazzier" T-shirt, which is available at lower cost than the earlier editions. Spectroscopists really have more fun, so get your T-shirt now while the supply lasts.

Finally, I'd like to announce that the Coblentz Society will be 30 years old in 1984. In commemoration of that event, we are planning a gala affair at the FACSS Con-
Moreover, as software goes further down the learning curve, its bug content will decrease, but eventually so does the level of support available for debugging operations.

The problem is one we have encountered before, when computer hardware problems were still a significant problem. Here the eventual solution was based on redundancy and internal checking. A similar approach would clearly be appropriate for spectroscopic software as well.

However, it is not quite clear how to do it. Internal checks can be easily defeated by the combination of unusual circumstances and of data for which the "reference truth" is not well known. The obvious approach here is to test software on "synthetic data" which appropriately tests the algorithms. Here the very large number of degrees of freedom in spectroscopic data means a factorially growing number of experiments, which quite rapidly becomes unrealistic. Nevertheless, the power of the computer can be harnessed to solving this problem by developing exerciser programs, which use all the available spare time to test algorithms over as much as possible of their operating envelope (the resemblance of this to dreaming may not be a coincidence).

More effectively however, it is possible to extend the concept of redundancy to software by having more than one independently developed algorithm to get from one point to another. Clearly one is talking here about fairly complex processes, in which more than a single path to a solution exists. While this is wasteful of both computer power and programming effort, technological advances and market increases are making this approach affordable.

Even while improvements are possible, this problem will continue to exist. All that will happen as we get better at eliminating bugs is that the remaining ones will be getting even more sophisticated, until they eventually merge with the reasoning errors characteristic of a human operator. In the meantime, suspecting everything is the only sane policy.

Pardon me, I've got to go now. The little green men from Mars that case me are at it again.

SPECTROSCOPIC FORECASTS

1. Hirschfeld

Paranoia is a Useful Trait. In this day and age of computer-controlled instruments, optional and not-so-optional computerized data treatment, computer-searched digitized data bases, and so on, it pays to think a little about preventing an uprising by our mechanical friends.

A computer is nothing but an extremely fast moron, capable of not only a million decisions but also a million mistakes a second. Given a tendency to use computers for quite substantial tasks, whose step-by-step verification is a once-only effort, mistakes usually surface only after many further generations of further processing; at this point they are often unrecognizable and usually quite hard to trace.

It is true that most computer errors are usually software ones and traceable to human error in programming. While straightforward programmer mistakes can usually be neutralized by double-teaming and comparison of the results, many higher order programming errors tend to give repeatable mistakes that cannot be detected in this fashion. The classical version of this is the failure by programmers to completely foresee all possible combinations of circumstances in which the program must work. Here operating experience, while a good bug-hunting procedure for the more frequent or serious problem, shows an exponential decrease in effectiveness with time. Eventually, as time passes, bugs become less frequent, but they never cease completely.

The problem is probably much worse than it looks. On one hand, our ability to detect bugs depends on their being clearly recognizable, which usually means catastrophic or nearly so. The fairly likely outcome of non-catastrophic failure will in many cases go unrecognized.
NOMINATIONS FOR THE BOARD
Nominations to the Board of Managers of the Coblenz Society are now open. Candidates should be members of the society with an interest in advancing the science of molecular spectroscopy and a willingness to contribute. The term of office is four years of rewarding experience and conversation regarding a subject of interest to all members. Nominations should be sent to:

Dr. R. J. Obremski
Beckman Instruments, Inc.
P.O. Box C-19600
Irvine, CA 92713

All nominations received by September 30, 1984, will be considered by the committee.

WILLIAMS-WRIGHT AWARD FOR INDUSTRIAL VIBRATIONAL SPECTROSCOPY THE COBLENTZ SOCIETY

NAME:
This award is named the Williams-Wright Award for Industrial Vibrational Spectroscopy. It has been established to honor the contributions of the (late) Van Zandt Williams, The Perkin-Elmer Corporation, and Norman Wright, the Dow Chemical Corporation.

SPONSOR:
The award is presented annually by the Coblenz Society. It consists of a lettered award certificate specifying the contributions made by the awardee (Dean Jim Durig, University of South Carolina, is the contact for preparing the award certificate).

CONDITIONS FOR THE AWARD:
The award is to be given to a person who has made significant contributions to vibrational spectroscopy while working in industry. The work may include infrared and/or Raman spectroscopy, instrumental development as well as theory and applications of vibrational spectroscopy. No restriction is placed on the selection of the awardee because of age, sex, or nationality, but the awardee must be still working at the time the award is presented. (Government labs are not considered industry in this definition.)

NEW BOARD MEMBERS

Robin S. McDowell
Robin S. ("Rod") McDowell received his B.A. from Haverford College in 1956 and his Ph.D. from M.I.T. in 1960 with Professor Richard C. Lord. He has been employed since then at Los Alamos National Laboratory as Staff Member, Assistant Group Leader of the Laser Photochemistry Group, and currently as Laboratory Fellow. His professional interests are in infrared and Raman spectroscopy (especially high-resolution Doppler-limited and sub-Doppler spectroscopy with use of tunable lasers), spectra of inorganic and isotopically substituted molecules, analysis of rovibrational energy levels, development of molecular lasers, and analytical techniques. He has authored or co-authored eighty-five papers in these areas, plus several review articles on infrared laser spectroscopy. A member of the Coblenz Society since 1965, he has served on several committees and is currently Chairman of the Coblenz Award Committee and a member of the Board Advisory Group. He also belongs to AAAS, OSA, Sigma Xi, the Society for Applied Spectroscopy, and the Laser Institute of America (Chairman, Los Alamos Chapter, 1979–80). He is active in the Los Alamos Optical Society and co-edited the Proceedings of the Los Alamos Conference on Optics '81 (SPIE Proc. 380) in addition to giving a short course on infrared laser spectroscopy at the conference. He feels that the Coblenz Society should continue to serve dispersive and FT-IR spectroscopists, but without neglect of such developing infrared techniques as laser and non-linear spectroscopy.

Laurence A. Nafie
Laurence A. Nafie received a B. Chem. degree with honors from the University of Minnesota in 1967 and a M.S. in Physics from the University of Oregon in 1969. After spending two years in the U.S. Army at the Nuclear Effects Laboratory, Edgewood Arsenal, Maryland, he returned to the University of Oregon and received a Ph.D. in chemical physics in 1973. His thesis work with Professor Warner L. Petiolas dealt with the theoretical formulation and interpretation of laser Raman scattering. From 1973 until 1975 Dr. Nafie was a postdoctoral associate with Professor Philip J. Stephens at the University of Southern California where, in the fall of 1974,
he verified the discovery of vibrational circular dichroism from individual molecules. In September 1975 Dr. Nafie was appointed to the Faculty at Syracuse University as an assistant professor. In 1979 he was promoted to associate professor and in 1982 to professor. In July of 1984 he will become Chairman of the Department of Chemistry at Syracuse University.

Professor Nafie's research program has as its principal goal the experimental and theoretical development of the new field of vibrational optical activity which is comprised of infrared vibrational circular dichroism and Raman optical activity. The major achievements of his research program are: (1) the first vibrational circular dichroism studies of amino acids and peptides; (2) the formulation of the localized molecular orbital model of vibrational circular dichroism intensities, including its first application and comparison to experiment; and (3) the development of infrared Fourier transform vibrational circular dichroism and its first observation with use of a new measurement procedure known as double modulation Fourier transform spectroscopy. In 1978 Dr. Nafie was awarded an Alfred P. Sloan Foundation Fellowship and in 1981 he was the Coblentz Society awardee. His research to date has resulted in over sixty scientific publications and, in addition to membership in the Coblentz Society, Dr. Nafie is a member of the American Chemical Society, the American Physical Society, the Optical Society of America, and the Society for Applied Spectroscopy. For the past year Dr. Nafie has served the Coblentz Society as a member of the Advisory Group.

INTERNATIONAL CONFERENCE ON FOURIER AND COMPUTERIZED INFRARED SPECTROSCOPY

The 1985 International Conference on Fourier and Computerized Infrared Spectroscopy will be held 24–29 June, 1985 at Carleton University in Ottawa, Canada. This is the fourth of a series of conferences which began in 1977 at the University of South Carolina. The conference will feature plenary and invited lectures in the morning, and poster sessions of contributed papers in the afternoon. Equipment displays and demonstrations as well as a full social program are planned.

Topics include: near-IR, correlation transform, high resolution and time-resolved spectroscopy; hyphenated methods (GC-IR, LC-IR, TLC-IR, etc.); sampling techniques; data processing; and applications in diverse fields. A special session, “What's New in Instrumentation?” will cover Fourier transform as well as computerized dispersive spectrometers.

Contributed papers for the poster sessions are solicited on all aspects of computerized infrared spectroscopy.

Convenient and economical accommodations will be provided in Carleton University residences, mostly in shared rooms. Downtown hotels are also available.

The Conference is sponsored by the National Research Council of Canada and co-sponsored by the Coblentz Society, the Optical Society of America, the Society for Applied Spectroscopy, the Spectroscopy Society of Canada, and the Society of Photo-Optical Instrumentation Engineers.

The General Chairman of the Conference is Dr. Tomas Hirschfeld, and the Program Chairman is Dr. Jeanette Grasselli. For further information, write Mrs. L. Baignee, Conference Services Office, National Research Council of Canada, Ottawa, Ontario K1A 0R6.

FORMAT FOR CALL FOR PAPERS

The 1985 International Conference on Fourier and Computerized Infrared Spectroscopy will be held 24–29 June 1985, at Carleton University in Ottawa, Ontario. Original papers for presentation in poster sessions are solicited on all aspects of computerized infrared spectroscopy, including acquisition, processing, analysis, sampling, interpretation of data and advances in instrumentation. Authors who wish to present papers at the 1985 Conference must submit a title by November 1, 1984 to Dr. Jeanette G. Grasselli, The Standard Oil Company (Ohio), 4440 Warrensville Center Road, Cleveland, OH 44128, U.S.A.

FORMAT FOR CALENDAR NOTICES

June 24–29, 1985 International Conference on Fourier and Computerized Infrared Spectroscopy, Carleton University, Ottawa, Canada. The General Chairman of the Conference is Dr. Tomas Hirschfeld and the Program Chairman is Dr. Jeanette Grasselli. For further information, write Mrs. L. Baignee, Conference Services Office, National Research Council of Canada, Ottawa, Ontario K1A 0R6.