THE COBLENTZ SOCIETY

NEWSLETTER

No. 118

A Society for Applied Spectroscopy Affiliate
Editor: K. S. Kalasinsky

February 1994

EDITOR'S COMMENTS

As you can see from this newsletter, this is becoming your news corner. Many spectroscopy events are happen- ing in 1994, and several of them are highlighted in this issue of the newsletter. You are welcome to contribute articles and comments on those items or events that you wish to publicize. The next due date for newsletter submissions is May 1st for the August issue. Regardless of the number of contributions, we will always be covering the events and progress of the Society so you can keep in touch with the board members and officers. Newsletter requests can be mailed directly to me as editor of the newsletter (Dr. Kathryn S. Kalasinsky, Armed Forces Institute of Pathology, Division of Forensic Toxicology, Washington, DC 20306). Be sure to look for the COBLENTZ Society Newsletter in every February and August issue of Applied Spectroscopy.

KATHY KALASINSKY

PRESIDENT'S MESSAGE

The 1993 fall meeting of the Coblentz Board of Man- agers was held in August at the University of Calgary, Alberta, Canada, site of the 9th International Conference on Fourier Transform Spectroscopy. This is most likely the first meeting of the Coblentz Board to have been held outside the United States of America—a truly historic event! Also of historic interest is the fortieth anniversary of the founding of the Coblentz Society. The Society has already celebrated this occasion at PittCon '93 in Atlanta, Georgia, with a symposium entitled "Fortieth Anniversary of the Coblentz Society: Historical Perspectives and Current State of the Art in Vibrational Spectroscopy." This year we are selling a limited-edition collector's-item version of our fast-moving Coblentz Society T-shirt, which comes in a new royal blue color and announces the fortieth anniversary. These shirts are available from the Society for $10 each. We have some newly designed flyers which highlight the Society, answer questions, and provide a membership application form. We are also planning to update the pamphlet, published ten years ago, that provided a historical summary of the Society and commemorated its thirtieth anniversary.

The most serious issue facing the Coblentz Society is financial stability. Sources of income to the Society, which allowed us to build financial reserves and initiate new activities in the 1980s, have dwindled sharply in the last several years. Given our modest membership dues, the Society must secure new sources of income or risk losing our ability to support worthy causes and scientific meet- ings in the future. The Board of Governors is presently

Chairman of the Lippincott Award Selection Committee, Kathy Kalasinsky (R), presents the Lippincott Award honorarium check to an elated Lippincott awardee, John Rabolt, at the International Fourier Transform Spectroscopy Conference held in Calgary, Canada, this past August. Session Chairman, Jerome Swalen, looks on.

Coblentz Society President, Larry Nafe (R) presents the Coblentz Award to Peter Felker of UCLA at the Ohio State Molecular Symposium in Columbus this past June.
working on new approaches to financial stability and new ways to make the Society more attractive to vibrational spectroscopists in all areas. We are currently working on a bulletin to be issued semi-annually and a booklet on sample handling.

I am pleased to report the results of our most recent awards. The Coblentz Award for 1993 was won by Professor Peter Felker of UCLA. The award was presented this past June at the Molecular Spectroscopy Symposium at the Ohio State University in Columbus, Ohio. Dr. John Chalmers of ICI Materials in the United Kingdom is the 1994 winner of the Williams–Wright Award, and Dr. Hector Casal of DCH Analysis, Inc. in Cleveland has arranged a symposium for PittCon '94 in Chicago. The 1994 Bomem–Michelson Award was won this year by Professor Herbert Strauss of the University of California, Berkeley. The award symposium for PittCon '94 has been arranged by Dr. David Cameron, also of DCH Analysis, Inc. Finally, this year, the Coblentz Society sponsored the Lippincott Award, which was won by Dr. John F. Rabolt of the IBM Almaden Research Center in San Jose, California. John Rabolt is the only person to have won three of the Society's four awards. Previously, he received the Coblentz Award (1985) and the Williams–Wright Award (1990). Keep up the good work, John!

Finally, in this, my first message to the Coblentz Society as President, I would like to thank our Past-President Rachael Barbour for a job well done and all the members of the Society for their many continuing contributions, even if it is only (for now) being a regular member. The Coblentz Society has the clear goal of supporting and promoting the science of vibrational molecular spectroscopy. If you would like to actively assist us in the endeavor, you are more than welcome to let us know and to volunteer your services.

Laurence A. Nafie

COBLENTZ SOCIETY PITCON GIVEAWAY

The Coblentz Society will have a booth at PittCon, to be held in Chicago this year. We will be soliciting memberships, displaying our data bases, and distributing order forms for our reference collections. Come by the booth to check our sponsoring events schedule. If you own a Coblentz Society Desk Book of the reference book Halogenated Hydrocarbons, we will give you new free dust covers for those books. Just stop by our booth and pick up your dust jacket! Also check out our new 40th anniversary T-shirts, which will be on display.

CALIBRATION STANDARDS FOR INFRARED INTENSITY MEASUREMENTS ON LIQUIDS

Infrared wavenumber calibration standards were established in the mid-1950s by the Commission on Molecular Structure and Spectroscopy of the International Union of Pure and Applied Chemistry (IUPAC). Together with subsequent revisions and extensions, these wavenumber standards are now approved for international use by the International Council of Scientific Unions (ICSU).

The situation concerning the measurement of infrared intensities is lamentably different, and only recently has an attempt been made to establish intensity standards comparable to the wavenumber standards. At its General Assembly in 1983, IUPAC set up a Working Party on Secondary Standards for Intensity Measurements in Infrared Spectroscopy. This international group, with R. Norman Jones as chairman and John Bertie as secretary, comprised nine members and thirteen collaborators, with representation from Australia, Canada, Germany, Hungary, The Netherlands, the Republic of South Africa, The U.K., and the U.S.A.

The Working Party reported to the IUPAC Commission at its biennial General Assemblies at Lyon (1985), Boston (1987), Lund (1989), and Hamburg (1991). It concentrated on standards for the measurement of analytical spectra in the liquid phase and published a technical progress report in Applied Spectroscopy in 1991. At the most recent IUPAC General Assembly at Lisbon last August, the Working Party formally proposed as intensity standards forty-two bands selected from the spectra of benzene, toluene, monochlorobenzene, and dichloromethane. These were approved by IUPAC and are currently in the hands of the IUPAC Committee on Publications. They were selected from a data base of 786 bands in the spectra of 13 liquids, covering the wavenumber range 4669 to 685 cm$^{-1}$ at pathlengths in the range 2 to 5000 $\mu$m.

The spectra are displayed, tabulated at 0.5-cm$^{-1}$ intervals, and three intensity quantities are listed in parallel columns. Of principal relevance to analytical spectroscopists is the molar decadic absorption coefficient $E_m$ where $E_m = A/Cd$, in which $A$ is the absorbance, $C$ the molar concentration in units of mole L$^{-1}$, and $d$ the pathlength (cm). Also tabulated are the real and imaginary components of the complex refractive index, $n$ and $k$. These quantities are derived directly from Maxwell's equations for the electromagnetic field and are of primary relevance to theoretical spectroscopists.

For analytical purposes, the Working Party strongly recommends that band areas between specific integration ranges be used rather than peak values, and such areas and integration ranges are incorporated into the stan-
The accepted values for the intensities are based on a statistical analysis of numerous measurements made by the members and collaborators of the Working Party in different laboratories with the use of FT-IR spectrometers of different manufacture. The estimated accuracy is better than 3% for $E_m$ and $k$, better than 0.2% for $n$, and better than 2% for the area measurements. Following the earlier experience with the Wavenumber Tables, it is to be anticipated that, as more data accumulate, the accuracy will improve, and from time to time the tables will be revised.

The Working Party recognized quite early that there is a problem in ensuring that different laboratories will use the standards in a consistent manner. Accordingly, incorporated into the standards specifications is a computer program IRYTRUE, a description of which has been published. Basically IRYTRUE evaluates a “cell constant” that adjusts for several operational differences which our experience has shown are liable to occur when measurements made in different laboratories and on different instruments are compared. This cell constant is to be used in place of the cell pathlength which enters into the algorithms used in quantitative infrared analysis of liquid samples. Use of this IRYTRUE program is part of the approved calibration procedure, and it will be incorporated, probably as a 3½-in. disk in the formal IUPAC publication.

R. Norman Jones and John E. Bertie
University of Alberta

10TH INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY

The 10th International Conference on Fourier Transform Spectroscopy will be held August 27 to September 1, 1995, in Budapest, Hungary. The scope of the conference comprises any aspects of Fourier transform spectroscopy in the infrared, far-infrared, visible, and ultraviolet regions, including Fourier transform Raman spectroscopy. Topics will range from fundamental aspects of theory (via experimental techniques and new methodology and development) to analytical methods of data and treatment. If you are interested in more information, please contact Prof. Dr. Janos Mink, University of Veszprem, Department of Analytical Chemistry, H-8201 Veszprem, P.O. Box 158, Hungary, or contact, Conference Office Secretary, Mr. Attila Varga, H-1371 Budapest, P.O. Box 433, Hungary. The next circular with the call for papers is scheduled for May 1994.

REQUEST FOR NOMINATIONS

The Coblentz Society requests nominations for the prestigious awards it supports:


1995 Williams–Wright Award. This award is presented annually at the Pittsburgh Conference to an industrial spectroscopist who has made significant contributions to vibrational spectroscopy while working in industry. The work may include infrared and/or Raman spectroscopy and instrumental development as well as theory and applications of vibrational spectroscopy. (Government labs are not considered industry in this definition.) No restrictions are placed on the selection of the awardee because of age, sex, or nationality, but the awardee must still be working at the time the award is presented. The nominating document should clearly state the significance of the contribution made by the nominee, i.e., the introduction of novel methods, techniques, or theories; innovative work in the field of vibrational spectroscopy; or significant vibrational spectroscopy arising from the volume of contributions in a specific area. The nomination should include a current vitae on the nominee and highlight any publications and talks. Seconding letters to the nomination are useful, but not necessary. Files on nomi-

Like the Coblentz Award, the prize includes a $1,000 cash prize plus a travel allowance to the Pittsburgh Conference. Nominations should be sent to the chairman of the Williams-Wright Award Selection Committee, Dr. Bruce Chase, CR&D 328/131A, Experimental Station, E. I. du Pont, Wilmington, DE 19898, Ph: (302)695-4434 on or before April 1, 1994.

1995 Bomem-Michelson Award. This award is dedicated to the memory of Professor A. E. Michelson, developer of the Michelson interferometer. Bomem sponsors the award to honor scientists who have advanced the technique(s) of vibrational, molecular, Raman, or electronic spectroscopy. Contributions may be theoretical or experimental, or both. The recipient must be actively working and may be associated with the academic, industrial, governmental, or private sector. The awardee must be 37 years or older. The award consists of a medal and an honorarium. The presentation will be made at the Pittsburgh Conference in March 1995.

In order to ensure that the award is based on an independent evaluation of the candidate's performance, the selection is made by a committee chosen by the Coblentz Society. A nominating letter and seconding letters should be sent to: Dr. Richard Dulhuy, Department of Chemistry, University of Georgia, Athens, GA 30602, Ph: (404)542-1950. The candidate's CV should be included as well as specific research efforts which make the candidate eligible for this award. Nominations will close April 1, 1994.


Ellis R. Lippincott Award. The purpose of the Ellis R. Lippincott Award is to honor Dr. Lippincott's memory by the recognition of significant contributions and notable achievements in the field of vibrational spectroscopy. The medal is sponsored jointly by the Coblentz Society, the Optical Society of America, and the Society for Applied Spectroscopy. It is awarded annually at an appropriate scientific meeting. The award consists of the medal and travel allowance to the meeting. The awardee will present an address related to contributions for which he/she is being honored. In addition there may be a symposium of talks by invited speakers.

Recipients of the medal must have made significant contributions to vibrational spectroscopy as judged by their influence on other scientists. Because innovation was a hallmark of the work of Ellis R. Lippincott, this quality in the contributions of the candidates will be carefully appraised. The contributions may be theoretical or experimental or both, and may have been made in the course of applied as well as basic research.

No restriction is placed on the citizenship or national origin of candidates. A candidate need not be a member of any of the sponsoring societies. The award will not be made posthumously unless an awardee should die after the procedure of selection has been completed.


Nominations should include the name and affiliation of the nominee and sufficient background information to justify the nomination. A nominator is expected to believe strongly enough in the quality of the work or her/his candidate to provide evidence for that belief. No restriction is placed on who may nominate, and all nominations received by the committee prior to May 1 in any given year will be considered for the award to be presented in the fall of that year or spring of the following year. Files on nominees are kept active for three years, after which the candidate must be renominated with an updated file or the file will be closed. Nominations should be submitted to: Chairman, Lippincott Award Selection Committee, % Optical Society of America, 2010 Massachusetts Ave., N.W., Washington, DC 20036, Ph: (202)416-4100.

SOCIETY ANNOUNCEMENTS
Membership. Anyone wishing to join the Society may do so by sending $10.00 to Dr. James A. de Haseth, Coblentz Society Membership Chairman, Department of Chemistry, University of Georgia, Athens, GA 30602.

Board Meeting. The Coblentz Society Board will hold its semi-annual meeting the first week in March at the Pittsburgh Conference in Chicago. Any article of business that you want the Board members to consider needs to be sent in writing to Dr. Laurence A. Nafe, Coblentz Society President, Department of Chemistry, 1-014 Center for Science and Technology, Syracuse University, Syracuse, NY 13244-4100, prior to the conference.

Annual Meeting. The annual meeting of the Coblentz membership will be held prior to the Williams-Wright Symposium at the Pittsburgh Conference. Be sure to attend, since the general business of the Society will be conducted.
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<tr>
<th>Name</th>
<th>Position</th>
<th>Address</th>
<th>Telephone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr. Matthew A. Harthcock</td>
<td>President</td>
<td>The Dow Chemical Company, 1897D Building, Midland, MI 48667</td>
<td>(517)636-6332</td>
</tr>
<tr>
<td>Dr. Curtis Marcott</td>
<td>Secretary</td>
<td>Procter &amp; Gamble, P.O. Box 398707, Miami Valley Labs, Cincinnati, OH 45239-8707</td>
<td>(513)245-2806</td>
</tr>
<tr>
<td>Dr. Richard A. Dluhy</td>
<td>Treasurer</td>
<td>Department of Chemistry, University of Georgia, Athens, GA 30602</td>
<td>(404)542-1950</td>
</tr>
<tr>
<td>Dr. Laurence A. Nafie</td>
<td>Immediate Past President</td>
<td>Department of Chemistry, 1-014 Center for Science &amp; Technology, Syracuse University, Syracuse, NY 13244-4100</td>
<td>(315)443-4109</td>
</tr>
<tr>
<td>Dr. David M. Haaland</td>
<td></td>
<td>Division 1823, Sandia National Labs, Albuquerque, NM 87185</td>
<td>(505)844-5292</td>
</tr>
<tr>
<td>Dr. John E. Bertie</td>
<td></td>
<td>Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2G2, Canada</td>
<td>(403)492-3560</td>
</tr>
<tr>
<td>Dr. Richard A. Palmer</td>
<td></td>
<td>Department of Chemistry, Duke University, Durham, NC 27706</td>
<td>(919)660-1539</td>
</tr>
<tr>
<td>Dr. Donald Kuehl</td>
<td></td>
<td>Galactic Industries Corp., 395 Main Street, Salem, NH 03079</td>
<td>(603)898-7600</td>
</tr>
<tr>
<td>Dr. David Schiering</td>
<td></td>
<td>Perkin-Elmer Corporation, 50 Danbury Road M-S 240, Wilton, CT 06897</td>
<td>(203)761-2915</td>
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**COBLENZ SOCIETY OFFICERS**

- **President:** Dr. Laurence A. Nafie  
  Department of Chemistry  
  1-014 Center for Science & Technology  
  Syracuse University  
  Syracuse, NY 13244-4100  
  (315)443-4109

- **Secretary:** Dr. David Schiering  
  Perkin-Elmer Corporation  
  50 Danbury Rd. M-S 240  
  Wilton, CT 06897  
  (203)761-2915

- **Treasurer:** Dr. Bruce Chase  
  CR&D 328/131A  
  Experimental Station  
  E. I. du Pont  
  Wilmington, DE 19898  
  (302)695-4344

- **Immediate Past President:** Rachael L. Barbour  
  BP Research  
  4440 Warrensville Center Road  
  Cleveland, OH 44128-2837  
  (216)581-5562