

NEWSLETTER

No. 124

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

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Coblentz Society President, John Bertie (L), presents the Coblentz Award and the traditional Coblentz prism to Xiaoliang Sunney Xie of the Pacific Northwest National Laboratory at The Ohio State Molecular Symposium in Columbus this past June.

EDITOR'S COMMENTS

Coblentz President John Bertie has made my job easy. The President's Message is very complete and covers all the events of the Society. It could stand alone as a newsletter. John has served the society well for almost two years now, and we will miss him as he steps down from his presidency in March. We look forward to the role that Arlene Garrison will be filling as our next president. You will be hearing from her beginning with the 1998 newsletters.

The Coblentz Society continues to grow and expand. This newsletter is your link with the rest of the society. You are welcome to contribute articles and comments for those items or events that you wish to broadcast. The next due date for newsletter submissions is May 1st for the August issue. Regardless of the number of contributions, we will always be printing the events and progress of the Society so that you can keep in touch with the board

members and officers. Newsletter requests can be mailed directly to the newsletter editor as noted in the officer section at the end. Be sure to look for the *Coblentz Society Newsletter* in every February and August issue of *Applied Spectroscopy*.

KATHY KALASINSKY

PRESIDENT'S MESSAGE

This is one of two times in the year when I as President have to remind myself about what has happened to your Society in the roughly six months since the last report and about the main issues that affect your Society and should be drawn to your attention. I remind you that you should now all be receiving your own copy of the newsletter mailed to your address. If you are not receiving it, please let Kathy Kalasinsky know. I should also tell you that your Society is holding its own financially in these difficult times, helped as always by the work of Clara Craver in selling the Coblentz books of spectra.

One important matter that I must remind you of is that



Coblentz Society President, John Bertie (L), presents the Lippincott Award to Giacinto Scoles of Princeton University at The Ohio State Molecular Symposium held this past June.



Arlene Garrison (L), President-Elect of the Coblenz Society, and John Bertie (R), current President, confer at the last Coblenz Board meeting held in Kansas City at the FACSS meeting.

Don Kuehl and David Schiering leave the Board of Management after Pittcon in March 1997. The ballots for their replacements were sent out with the dues notices, and I hope you voted. In Fall 1997 we shall be seeking nominations for board members to replace Robin Garrell and Nancy Ferris, whose terms end at Pittcon 1998. Now is a good time to start thinking about nominating the people you would like to see on the Board of Managers of your Coblenz Society.

At Pittcon the annual membership meeting of your Society was held bright and early at 8:30 am on Tuesday morning. Each year this meeting precedes the Williams–Wright Symposium, and it gives all members the opportunity to hear about, and to ask about, the activities of the Society.

Following the annual membership meeting, I had the pleasure of presenting the Williams–Wright Award to Bob Messerschmidt for his outstanding contributions to the art and science of spectroscopic accessories. Bob has reduced the strain on many scientists through his creation of accessories that solve their problems. Bob spoke about the science of his career, as well as embarrassing as many people as he could in the time available with his reminiscences about their less illustrious moments. It was an entertaining and informative talk. Bob was followed in the Williams–Wright Symposium by John Reffner, Neil Lewis, Jack Koenig, and Carl Zimba, who presented different and very impressive aspects of infrared microscopy and imaging and thus contributed to an extremely well-attended and well-received symposium. The credit for organizing this symposium is due to Richard Palmer.

Again following tradition, the Williams–Wright Symposium was followed by the annual wine and cheese mixer. This is a delightful, relaxed event at which a little wine is drunk and some cheese and goodies are eaten, but the main pleasure is getting to meet old friends again and getting to know the younger and newer members of the Society. If you have not come to the “Coblenz Wine and Cheese” at Pittcon yet, please do come and say Hi. You will make and meet lots of friends.

The Wednesday afternoon at Pittcon saw another very successful Coblenz Society symposium, the Bomem–Michelson Award Symposium, which is sponsored by Bomem Inc. of Quebec, Canada. A committee of the Coblenz Society selects the winner of this award, and Henry Buijs of Bomem presents the award and very generously pays



Long-time Coblenz member and outstanding contributor to molecular spectroscopy, Abe Savitsky, was presented with honorary membership in the Society of Applied Spectroscopy at the FACSS conference in Kansas City this past October. Abe is shown here with his wife, holding the award plaque.

the bills. Your President and Board of Managers value and appreciate Henry’s generosity immensely, and equally value and appreciate the complete trust he places in the Coblenz Society to ensure that the high caliber and reputation of the award are continually enhanced.

In February 1996 the caliber and reputation of the award were certainly enhanced, because Henry had the pleasure of presenting the award to Ira Levin and then hearing Ira’s fascinating account of the contributions that vibrational spectroscopic and imaging studies have made to our knowledge of the domain architecture of biological membranes. Ira was followed by Bruce Chase, John Rabolt, and Peter Griffiths, who gave impressive illustrations of how vibrational spectroscopy is of real importance in very sophisticated monitoring of production samples in the polymer industry, in the development of sophisticated surfaces for the computer industry, and in the analysis of samples from the “real world”. John Hellgeth organized this superb and very well-attended symposium. The symposium finished early, with the last scheduled speaker, Bill Harris of NSF, still circling the skies above Chicago because, as an Assistant Director of the National Science Foundation, he has to give the business of an important United States Congressional Committee precedence over a scientific symposium.

Three other awards of the Coblenz Society have been presented for distinguished science in the past six months. At the 51st International Symposium on Molecular Spectroscopy in Columbus in June, I had the pleasure of presenting two of them.

First was the Lippincott Award, which is jointly sponsored by the Optical Society of America, the Society for Applied Spectroscopy, and the Coblenz Society. The



Spectroscopists Bob Jakobsen (L), John Bertie (Coblentz President), and Jimmy Brash (R) enjoy themselves at one of the many social functions at the FACSS conference in Kansas City this past October.

three societies take it in turns to host the award. In June, I acted on behalf of the Society for Applied Spectroscopy to present the 1995 Lippincott Award to Giacinto Scoles of Princeton University. Symposium organizer Terry Miller and his program committee placed this event first on their program, and following the presentation Giacinto gave the first plenary lecture of the symposium, his Lippincott Award lecture on the spectroscopy and dynamics of high-spin dimers and trimers of alkali metal atoms "matrix-isolated" in large helium clusters. It was a great start to a week-long symposium that was as strong as always.

Second, I presented the Coblentz Award for outstanding work by a molecular spectroscopist under age 36 to X. Sunney Xie of the Pacific Northwest National Laboratory. This presentation, followed by the Coblentz Award lecture, is a regular fixture at the end of the Monday morning session at Columbus. Sunney gave a very impressive and well-received lecture, "Single Molecule Spectroscopy and Chemical Dynamics at Room Temperature". The Coblentz Award is a highly prized honor whose stature increases each year.

In August, the 1996 Lippincott Award, for which the Coblentz Society was the host, was presented at Sandy Asher's successful International Conference on Raman Spectroscopy in Pittsburgh, which your Society assisted financially. John Rabolt kindly and very ably acted for me in presenting the 1996 Lippincott Award to Giuseppe Zerbi immediately before Gus's award lecture, which was also a plenary lecture to the conference titled "Hyperpolarizabilities of Materials Relevant in Molecular Electronics: A Spectroscopic Approach".

The annual cycle of awards starts again at Pittcon in Atlanta, March 16 to 21, 1997. The Williams-Wright Award will be presented to Michael Pelletier for his creative work on developments in Raman instrumentation, particularly the use of array detectors. Mike heads another impressive symposium arranged by Richard Palmer, which features Bruce Chase, Curt Marcott, Michael Morris, and Joel Harris. The annual business meeting takes place immediately before the symposium, and the Coblentz Society wine and cheese reception follows it. Plan to attend all three events at Pittcon '97 in Atlanta.

Also at Pittcon '97, the Bomem-Michelson Award will be presented to William (Woody) Woodruff for his development and application of time-resolved vibrational

spectroscopy. John Hellgeth has again arranged the symposium, with Gerald Babcock, Tom Spiro, and others supporting Woody. It will be a superb symposium on the application of advanced vibrational spectroscopic techniques to the dynamics of biological processes. Do not miss it in Atlanta.

Relations between the Coblentz Society and the Pittcon organization are very good, and Pittcon is very supportive of our symposia and general needs. The main problem we have experienced in recent years is the coincidence of other vibrational spectroscopy sessions with the award symposia. Pittcon's program chairs have been responsive to our difficulties, and I am pleased that the Williams-Wright and Bomem-Michelson symposia in Atlanta are at the same times as in Chicago, namely, on Tuesday morning and Wednesday afternoon, respectively. Maintaining the same time slot for these symposia should lead to fewer conflicts in the long run.

Another set of awards of importance to the Coblentz Society are its Student Awards. Rod McDowell coordinates these awards. Last year they were made to 14 students. They are Michael Bellamy of Kansas State University; Zhan Chen of the University of California, Berkeley; Christopher DiGiacomo of Case Western Reserve University; Bernd Dippel of Universität Essen, Germany; Stephanie Harris of Towson State University; Roseann Hoffman of Kansas State University; Helen Joo-On Kang of Wellesley College; Stephen Mahan of the University of Tennessee; David Manuel of Idaho State University; Matthias Pusch of Alfred University; A. J. Rossman of the Rose-Hulman Institute of Technology; Neil Silvesky of Farmingdale State University; Maria Vargek of Syracuse University; and Darren Williams of Oregon State University. Sincere congratulations and best wishes for future success go to all of these students.

The Society's database program has long been in the hands of Clara Craver, to whom the Society owes a tremendous debt of gratitude. The infrared spectral books have for years brought the Coblentz Society into laboratories around the world. They have also enriched the coffers of the Society, which is an important factor for a society that has very small membership dues and supports major programs of awards. The database program has been extended. Two years ago the Coblentz Society signed a Cooperative Research and Development Agreement (CRADA) with NIST to develop a digital database that will be marketed. Much progress has been made since then, including the conversion of many of the society's hard-copy spectra into digital form. Clara and Kathy Kalasinsky have worked very hard on this project, which is now at the stage that requires us to solicit spectra of authenticated samples from individuals and laboratories willing to donate them to the Society. If you have spectra of reliable samples, in either digital or hard-copy form, that you are willing to donate to the Society, please call Kathy Kalasinsky at phone (301)319-0055, fax (301)319-0628, or e-mail at the world's longest e-mail address, kalasink_at.afip04@email.afip.osd.mil. If you prefer to call Clara Craver, please do so at phone/fax (573)358-2589. It is planned that the digital database should be available for sale next fall, and we will keep members informed of progress.

The Coblentz Society sponsored the second Interna-

tional Symposium on Advanced Infrared Spectroscopy, i.e., AIRS II, which was held at Duke University in June. About 140 people attended. The conference was successful financially as well as scientifically, and your Society recovered its funds. In this way your Society can continue to supply significant seed money to important conferences on vibrational spectroscopy. Plan to attend the next conference in this series, the third International Symposium on Advanced Infrared Spectroscopy, or AIRS III, which will be held at the Vienna University of Technology, Austria, July 5th to July 9th, 1998. You can learn more about it from the web at <http://www.iac.tuwien.ac.at/~airsiii>.

The Society has also sponsored the 11th International Conference on Fourier Transform Spectroscopy, which Jim de Haseth and Rich Dluhy are organizing for Athens, Georgia, for August 10 to 15, 1997. Rich has a great program of invited speakers, and Jim has worked to provide food and accommodation at an affordable price, so make sure to go to Athens in August 1997. Learn more from the web site <http://dehsrv.chem.uga.edu/icof11/index.html>.

The Coblenz Society now has its own web site, largely through the work of Don Kuehl. It is currently situated at <http://www.alberta.ca/~jbertie/coblenz.htm>. It will be moved soon, but we will keep you informed and redirected. Visit our web site and let Don know what additional material you would like to see on it.

JOHN BERTIE

COBLENTZ/NIST JOIN EFFORTS TO PRODUCE IR DATABASE

The Coblenz Society and the National Institute of Standards and Technology (NIST) have joined efforts to produce a much-needed digital infrared database for spectral searching and identification. The Coblenz Society has long been noted for its high-quality evaluated infrared reference data and for the recommended standards for infrared data productions. NIST has long had the reputation of producing the highly circulated mass spectral database and is now entering a joint effort to likewise produce an infrared database. This new joint effort is initiated under a Cooperative Research and Development Agreement (CRADA) pursuant to 15 U.S.C. section 3710a. Under this agreement NIST and Coblenz will produce a digital infrared database for distribution through NIST as the *Coblenz/NIST IR Data Base*.

The initial product from NIST is targeted for an early 1997 release and will contain approximately 10,000 spectra. Approximately half of the spectra are from the NIST/EPA library and half are spectra from digitized Coblenz reference data. Initially the IR database will include both gas-phase and solid-phase spectra but will be broken down into subsets by phase and compound class once the database is sufficiently large to warrant such an arrangement. Specialty subsets of IR data much like the existing Coblenz reference volumes are on-line for production. The existing 10,000 spectra volume series of Coblenz data are also on-line for inclusion in the Coblenz/NIST IR database. Updates of the database are scheduled to be produced periodically.

NIST will be providing additional data measurements and database compilation for distribution including software developments for data handling. The Coblenz Society will be spearheading data solicitation and data evaluation. Any individuals or organizations that have produced IR reference data sets are encouraged to participate in this effort. The Coblenz Society will be collecting data sets and evaluating them for inclusion into the Coblenz/NIST IR database. Contributors may retain the copyright for donated spectra or assign the copyright to NIST or the Coblenz Society.

If you are interested in this database or contributing data to this national/international effort, please contact either Kathy Kalasinsky (301/319-0055) or Clara Craver (573/358-2589) for further information.

1997 INTERNATIONAL FTS CONFERENCE

The Eleventh International Conference on Fourier Transform Spectroscopy, ICOFTS-11, will be held in Athens, Georgia, August 10–15, 1997. This conference is sponsored by the Coblenz Society. The scientific program will consist of invited plenary lectures combined with daily contributed poster sessions. As in past conferences with the ICOFTS series, the scientific program will reflect a strong interdisciplinary emphasis involving the development and applications of Fourier transform spectroscopy. Topics to be covered will include advanced materials; analytical applications; atmospheric, astrophysical, and environmental chemistry and physics; biochemical and biophysical applications; chemometrics and data processing; fiber optics, sensors, and process control; FT-Raman spectroscopy; geological and mineralogical applications; high-resolution spectroscopy; methods development, advances in absorption, emission, reflection, hyphenated methods, matrix isolation, etc.; microscopy; molecular structure and dynamics; new emerging techniques; polymers and ordered systems; spectra imaging, including latest advances in array detector technology; step-scan frequency-domain and time-domain spectroscopy; surfaces and interfaces; time-resolved and transient phenomena; and UV-vis and NIR applications. Contributed papers are invited in all areas of Fourier transform spectroscopy. Abstracts are due by April 30th, 1997. Abstract forms will be available at the Coblenz Booth at the Pittsburgh Conference. Additional information can be obtained from

Professor James A. de Haseth
General Chairman, ICOFTS-11
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Athens, Georgia 30602-2556
Phone: (706)542-1968
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or browse the World Wide Web page at: <http://dehsrv.chem.uga.edu/icof11>.

CALL FOR NOMINATIONS FOR THE COBLENTZ SOCIETY'S AWARDS

Coblenz Award. The Coblenz Award is presented annually to an outstanding young molecular spectroscopist under the age of 36. The candidate must be under

the age of 36 on January 1 of the year of the award. Previous recipients of this award are: John Overend (1964), William Fateley/Robert Snyder (1965), Edwin Becker (1966), Peter Krueger (1967), Jon Hougén (1968), James Durig (1969), Guiseppi Zerbi (1970), Clive Perry (1971), George Leroi (1972), C. Bradley Moore (1973), C.K.N. Patel (1974), Bernard J. Bulkin (1975), Geoffrey Ozin/George Thomas, Jr. (1976), Peter Griffiths (1977), Lester Andrews (1978), Lionel Carreira (1979), Richard Van Duyne (1980), Laurence Nafie (1981), Christopher Patterson (1982), Dave Cameron (1983), Steve Leone (1984), John Rabolt/Graham Fleming (1985), Joel Harris (1986), Alan Campion (1987), Keith Nelson (1988), Geri Richmond (1989), Hai-Lung Dai (1990), Paul Bohn (1991), Thomas Rizzo (1992), Peter Felker (1993), A. Paul Alivisatos (1994), David J. Rakestraw (1995), and Xiaoliang Sunney Xie (1996). The award carries with it a \$1,000 prize plus a \$500 travel allowance. Files of candidates will be kept active until the date of age eligibility is exceeded. Annual updates of files of nominated candidates are encouraged.

Nominations, which should include a detailed description of the nominee's accomplishments, a curriculum vitae, and as many supporting letters as possible, must be submitted to the award chairman [Dr. John Hellgeth, Spectra-Tech, Inc., 2 Research Drive, Shelton, CT 06484-0869; phone (800)243-9186 (USA only) or (203)926-8998; fax (203)926-8909; e-mail hellgeth@spectra-tech.com] on or before July 1, 1997.

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, 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, e.g., the introduction of novel methods, techniques or theories; innovative work in the field of vibrational spectroscopy; significant improvement on existing methods, theory, or techniques; or important impact on the field of vibrational spectroscopy arising from the volume of contributions in a specific area. The nomination should include a resume of the nominee's career and should highlight the accomplishments and any publications and talks. Seconding letters to the nomination are useful but not necessary. Files on nominees will be kept active for three years, after which the candidate must be renominated with an updated file or the file will be closed.

Previous recipients of the Williams–Wright Award are: Norman Wright (1978), Norman Colthup (1979), Jeanette Grasselli (1980), Paul Wilks/James Harrick (1981), Robert Hannah (1982), Harry Willis (1983), Robert Jakobsen (1984), Clara Craver/Richard Nyquist (1985), Abe Savitsky/Joseph Barrett (1986), A. Lee Smith (1987), Darwin Wood (1988), Bruce Chase (1989), John F. Rabolt (1990), Bob Obremski (1991), Tim Harris (1992), Curtis Marcott (1993), John M. Chalmers (1994), Michael R. Philpott

(1995), Robert G. Messerschmidt (1996), and Michael J. Pelletier (1997).

The award includes a \$1,000 cash prize plus \$500 toward travel expenses to the Pittsburgh Conference. Nominations should be sent to the Chairman of the Williams–Wright Award Selection Committee [Dr. David Haaland, Sandia National Laboratories, MS 0342, Albuquerque, NM 87185-0343, phone and fax (505)844-5292; e-mail DMHAALA@SANDIA.GOV] before February 1, 1998.

Bomem–Michelson Award. This award is dedicated to the memory of Professor A. E. Michelson, developer of the Michelson interferometer. Bomem, Hartmann & Braun 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 at least 37 years of age. The award consists of a crystal symbol of the Bomem–Michelson award and an honorarium. In order to ensure that the award is based on an independent evaluation of the candidate's achievements, the selection is made by a committee chosen by the Coblenz Society. The presentation will be made at the Pittsburgh Conference in March 1998.

Previous recipients of the Bomem–Michelson Award are: Thomas G. Spiro (1987) W. Carl Linberger (1988), Richard J. Saykally (1989), William Klemperer (1990), Alan Pine (1991), Jyrki Kauppinen (1992), Jack L. Koenig (1993), Herbert L. Strauss (1994), Terry A. Miller (1995), Ira W. Levin (1996), and William H. Woodruff (1997).

The nomination should include a resume of the candidate's career as well as the special research achievements that make the candidate an eligible nominee for the Bomem–Michelson Award. Files on nominees will be kept active for three years, after which the candidate must be renominated with an updated file or the file will be closed. The nominating letter and supporting letters should be sent to: Dr. Nancy S. Ferris, Analytical Technology Division, Eastman Kodak Company, Rochester, New York 14650-2132; phone (716)722-0418; fax (716)477-7781. Nominations close March 31, 1997.

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 Coblenz 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 allowances to the meeting. The awardee will present an address related to the contributions for which he or 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 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 selection procedure has been completed.

Previous recipients include: Richard G. Lord (1976), Lionel Bellamy (1977), Bryce Crawford, Jr. (1978), E. Bright Wilson (1979), George C. Pimentel (1980), Ian Mills (1981), Michel Delhaye (1982), John Overend (1983), Jon T. Hougen (1984), Ira W. Levin (1985), Wolfgang Kaiser (1986), C. Bradley Moore (1987), Andreas C. Albrecht (1988), Marilyn E. Jacox (1989), Robert W. Field (1990), Richard J. Saykally (1992), John F. Rabolt (1993), Herbert L. Strauss (1994), Giacinto Scoles (1995), and Giuseppe Zerbi (1996).

Nominations should contain the name and affiliation of the nominee and sufficient background information to justify the nomination. A nominator is expected to believe sufficiently strongly in the quality of the work of his or her candidate to provide evidence of that belief. No restriction is placed on who may nominate, and all nominations received by the committee prior to May 1 in any year will be considered for the award to be presented in the fall of the following year. Files of nominees will be kept active for three years, after which the nominee must be renominated with an updated file or the file will be closed. Nominations should be submitted to: Lippincott Award Chairperson, Optical Society of America, 2010 Massachusetts Avenue, NW, Washington, D.C. 20036; phone (202)416 4110.

SOCIETY ANNOUNCEMENTS

Membership. Anyone wishing to join the Society may do so by sending \$10 to Dr. James A. de Haseth, Coblenz Society Membership Chairman, Department of Chemistry, University of Georgia, Athens, GA 30602.

Board Meeting. The Coblenz Society Board will hold its semi-annual meeting Monday, March 17th at 7:00 p.m. at the Pittsburgh Conference in Atlanta. Any article of business that you want the board members to consider needs to be sent in writing to Dr. John Bertie, Coblenz Society President, Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2, Canada, prior to the conference.

Annual Meeting. The annual meeting of the Coblenz membership will be held prior to the Williams-Wright Symposium Tuesday Morning, 8:30 a.m. at the Pittsburgh Conference. Be sure to attend, since the general business of the Society will be conducted.

Wine & Cheese. The Coblenz Society wine and cheese reception will be held at 12:15 p.m. Tuesday following Williams-Wright Symposium at the Pittsburgh Conference in Atlanta.

COBLENTZ SOCIETY BOARD

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Dr. Nancy Ferris Analytical Technical Division Eastman Kodak Company, Bldg. 82 Rochester, NY 14650-2132	1998	(716)722-0418
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