Coblentz Award

Dr. Peter R. Griffiths, Associate Professor of Chemistry at Ohio University, Athens, Ohio, has been named, as this year's recipient of the Coblentz Award.

This award is given annually to an outstanding scientist in molecular spectroscopy under age 36, and will be presented to Dr. Griffiths at the 1977 Pittsburgh Conference during the Coblentz Society Symposium on Thursday, March 3.

Dr. Griffiths earned his B.A., with first class honors in Chemistry at St. Johns College, Oxford; and his Ph.D. under the supervision of Sir Harold Thompson, also at Oxford. He then spent two years at the University of Maryland as a research associate with the late Ellis Lipplincott. Following a year as product specialist for FT-IR spectrometers with Digilab, Inc. in Cambridge, ..., and two years as manager for analytical services with Sadtler Research Laboratory in Philadelphia, PA, he joined the faculty of Ohio University, Athens, OH. His research interests center largely on development of analytical applications of FT-IR spectrometry.

President's Comments

Elsewhere in this newsletter, Jim Durig and I comment on the pros and cons of the CS-SAS affiliation. A ballot asking for your approval of the recommendations of the Board of Management of this affiliation has been enclosed along with the newsletter. I do not intend to make any further comments on this issue except to urge you to vote on this important issue and promptly return your ballot to Bob Hannah.

In past newsletters, I have commented on the problem of communication between the membership of the Society and the Board of Managers. This communication (or rather the lack of it) directly contributes to the way some people feel about the Society, and for some of the philosophy and aims of the Society. When the Board of Managers and the special committee have no communication from the membership, they have to act on their own concept of what is good for vibrational spectroscopy. Since all of us have special interests, and to a greater or lesser extent biased, this means that over a period of years the philosophies and work of the Society tend toward specialized areas (all good) but may not necessarily reflect the interest of the total spectroscopic world. Thus it is vitally important that we -- as members of the CS -- vote promptly on the enclosed ballot and attend and participate in the general membership meeting of the Society, Thursday afternoon at the Pittsburgh Conference. The Board of Management can only serve your interest if you tell them what you want.

Cleveland, 1977

Coblentz Award Symposium

2:00 Presentation of the 1977 Coblentz Award to Professor Peter R. Griffiths, Ohio University by Robert J. Jacobson, President Coblentz Society

Symposium: ANALYZING THE ATMOSPHERE BY INFRARED TECHNIQUES

Bernard J. Balkin, Chairman

2:15 Award Address: "Recent Applications of FT-IR Spectrometry in Chemical and Environmental Analysis." Peter R. Griffiths, Ohio University, Athens, Ohio

3:00 Recess

3:20 "Detection and Photochemistry of Selected Air Pollutants Using FT-IR Techniques," John Shaw, Ohio State University, Columbus, Ohio

3:55 "Opto-Acoustic Spectroscopy; Applications to Detection of Minute Concentrations of Gases," C. K. N. Patel, Bell Laboratories, Murray Hill, New Jersey
SAS AFFILIATION?

"PRO"

R. J. Jakobsen, President
The Coblentz Society

By a vote of 5 to 1, the Board of Management of the Coblentz Society (CS) has recommended that the Society follow the path of the Fourier Transform Spectroscopy (FTS) group and become a technical affiliate of the Society for Applied Spectroscopy (SAS). Obviously, the Board feels that there are many advantages in such a cooperative venture, but before going into these, I will mention several points:

1. Such an affiliation will not result in any loss of character or identity of the CS. The FTS group retains its identity and is free to carry out its programs and fulfill its purposes.

2. The CS would essentially become like the technical division of the American Chemical Society, free to handle its own internal affairs, and along with the FTS group, be responsible for the technical quality of the vibrational spectroscopy within the SAS. Indeed, the CS would have voting power within SAS (a delegate of the Governing Board of the SAS) and thus have some influence in the affairs of the SAS.

3. The aims or goals of the SAS and the CS are essentially the same; i.e., to promote and disseminate information about spectroscopy (specifically vibrational spectroscopy in the case of the CS).

With these points in mind, a very brief summary of the advantages of such an affiliation is listed below:

1. At the present time the CS does not serve vibrational spectroscopy as a whole, but only specific parts of vibrational spectroscopy. The Raman and FT-IR people felt that the CS did not fulfill their needs and formed separate groups. A Coblentz-SAS affiliation would insure closer cooperation between the CS and the FTS group (and perhaps lead to an assimilation of the FTS group by the CS). Like the CS, the Raman Technical Group is considering affiliation with the SAS. If this comes about, it would bring the Raman group and the CS closer together.

2. There are many vibrational spectroscopists in the SAS who are not members of the CS. These people would be much more likely to participate in the CS activities if the Society were affiliated with the SAS.

3. Two societies working toward the same goals can do more together than separately.

4. The CS can use the SAS journal to publicize and promote the CS.

5. The CS can continue to levy and collect its own dues and in addition will be able to solicit some financial assistance from the SAS when needed.

6. It has been argued that the SAS does not do much for the IR man. Yet the FTS group felt that the SAS could do more for it than the CS. In addition, when I personally surveyed the SAS and CS membership list: 45% of the people that I knew worked in IR were not members of the CS. This 45% must believe there is some value in the SAS.

For these reasons (and others), I strongly urge you to vote for affiliation of the CS in the SAS. Only with such affiliation can the CS begin to serve all of the vibrational spectroscopists instead of only specialized segments of this important area.

"CON"

J. R. Durig
Past President

I am opposed to the affiliation of the Coblentz Society with the Society for Applied Spectroscopy for the following reasons:

1. I believe the merger would dilute the Coblentz Society and would eventually result in an organization without identity. One of the purposes of the Coblentz Society was to foster a better understanding and applications of infrared spectroscopy between the industrial community and academic spectroscopists. It is my belief that the organization has been relatively successful in carrying out this aim. The Coblentz Society membership at present consists not only of applied spectroscopists, but also has a large contingency of people who did not fulfill their needs and formed other groups. The mixture of applied and "pure" infrared spectroscopy, if we may call it that, is exactly the admixture of personnel that originally founded this society. Loss of this broad scientific representation could minimize the effectiveness of the Society in certain matters.

2. The Coblentz Society has been able to be a semi-international organization. I would like to point out that we have members in Canada as well as in Europe. Affiliation with the Society for Applied Spectroscopy, which is an organization located wholly within the United States, would make the Coblentz Society more of a national organization. As a further point that the Coblentz Society is international, I should point out that at least two of our past recipients of the Coblentz Memorial Prize have been either Canadians or Europeans. Therefore, it is my sincere belief that affiliation would narrow the scope of our organization.

3. The Coblentz Society is a scientific group which is well recognized. We have successfully been arranging symposia at the PANSS and Pittsburgh Conference on Molecular Spectroscopy as well as the Ohio State Meeting on Molecular Spectra and Structure. Affiliation with SAS would not enhance our scientific image. I have spent four years on the Board of Directors, and I do not believe that the Coblentz Society would benefit from another layer of control. There is a great advantage to having an independent organization whose Board approves an item of business and no further approval is necessary. Such independence gives one great flexibility in pursuing the various courses of action, and I have always found that belonging to a larger group will eventually require some type of approval in the decision making process. I am speaking from my own experience as a university administrator in that we always seem to
eventually add another layer of control. Thus, I feel that the SAS may not immediately exercise its control, but in the long run it would be apparent.

I believe that Coblentz Society exercises a voice in the spectroscopic community that would not be as vocal or as apparent if we were a member of a larger organization. We have some very useful programs which potentially could suffer from this affiliation. I know for a fact that our Speakers' Bureau has enjoyed some success, and I recently was contacted to present a seminar at a local section of the American Chemical Society. Several of our programs have met with considerable success, and I am afraid that some of them would eventually suffer from such a merger.

5. I also feel that our organization would not be as functional as it currently is. We have had problems in the past, and I am afraid that the Board might simply give up and not be willing to spend the time and the energy to work out the problems of the organization if it were affiliated with the SAS. The Coblentz Society has been able to progress because of the exceptionally hard work of a limited number of people, but I feel that some of those individuals would not be willing to work as hard as they have in the past if we were a member of the larger organization.

6. I see no financial advantage to joining the SAS. The financial situation of the Coblentz Society is excellent at this time, and we can provide our membership with several benefits at a very minimal cost to members of the organization.

7. Finally, I would like to state that I feel the Society for Applied Spectroscopy is essentially a confederation of local sections and that many of the smaller groups, essentially, are doing what they want to. If the parent organization should become stronger, then I believe that it would limit a great deal of this flexibility. Similarly, SAS may exercise additional control on affiliated organizations, and I do not feel that the Coblentz Society, at this time, is willing to become subservient to the larger organization.

SPECTROSCOPIC VIBRATIONS

One of the more important instrumental innovations in infrared spectrometry is the development of the tunable diode laser spectrometer. These instruments enable spectra to be measured at extremely high resolution (0.0001 cm⁻¹), much higher than other commercially available infrared spectrometers. For example, a good grating spectrometer will allow spectra to be measured at a resolution of better than 0.2 cm⁻¹, while the best resolution for commercial Fourier transform spectrometers is of the order of 0.05 cm⁻¹ (although "homemade" spectrometers have attained two orders of magnitude better resolution than this in both cases).

Most tunable diode lasers for mid-infrared spectrometry are produced from lead salt semiconductor crystals such as PbI₂-xSn²P₂, PbS-xSex, PbxCd₁-xS, and even quaternary alloys. The alloy composition determines the wavelength region over which the diode lasers are tunable. Lasers are scanned over a range of approximately 1 cm⁻¹ by varying the current that powers them, and the nominal emission wavelength is varied by changing the temperature of the diode. The diodes are normally operated at a temperature between 10 K and 100 K, and a given diode is usually tunable over a maximum of between 50 cm⁻¹ and 300 cm⁻¹. The most convenient cryostat for cooling the diodes is the closed-cycle, Joule-Thompson type, since cryostats of this variety eliminate the necessity for a constant supply of liquid helium. The diodes are usually mounted in a low resolution grating monochromator to discriminate against emission lines other than the one of interest.

The most obvious application for these instruments, other than high resolution spectrometry for molecular structure research, is the monitoring of atmospheric pollutants. The narrow half-width and high power (often about 1 milliwatt) of the laser emission lines mean that measurements of very low sensitivity and specificity can be made, and the fact that the beam is highly collimated means that measurements can be made over long pathlengths. Hinkley and his coworkers at M.I.T. Lincoln Laboratories have measured the variation of carbon monoxide over highways as a function of traffic density. Hinkley, who recently gave a paper on recent developments in laser spectrometers at the Coblentz Society symposium at the FACSS meeting in Philadelphia, has pioneered many of the instrumental developments in this subject. He is now with Laser Analytics, Inc., of Lexington, Massachusetts, who manufacture these instruments.

It should be noted that commercial tunable diode laser spectrometers are not yet routine analytical instruments. They are single-beam instruments for which the customer has to develop his own way of converting the detector signal into a usable spectrum. These instruments appear to this author to be ripe for computerization. They are also quite expensive, since each diode costs may $3000 and may only cover a range of 50 cm⁻¹, so that several lasers are often required. Tunable laser spectrometers should therefore not even be considered for routine low resolution chemical spectrometry where wide tunability would be necessary. However they are ideally suited for several applications where high resolution measurements are needed over relatively short spectral ranges, and are most likely to see their greatest use in characterizing gas-phase or matrix-isolated samples.
The Fifth International Conference on Raman Spectroscopy was held at the University of Freiburg in West Germany from the 2nd to the 8th of September, 1976. There were over 400 attendees at the conference and the program was composed of six invited lectures of 45 minutes length and twenty invited papers of 25 minutes length. Additionally, there were 99 short communications of five minutes duration and 168 contributed papers with a length of twelve minutes each. The six invited lectures along with the twenty invited papers were abstracted with an average length of ten pages, and along with the 99 short communications and 168 contributed papers, which were abstracted to an average of two pages, were printed by direct offset. This attractive volume was available to the participants upon their arrival. The volume was approximately 800 pages long, and I am quite sure that the participants found it extremely valuable in making their decisions on what papers to attend. Because of the large number of contributed papers, it was necessary to run three parallel sessions. With the large number of Raman spectroscopists currently in the field, it will continue to be necessary at international meetings to have parallel sessions, and it is this reviewer's belief that the field is divergent enough that several sessions can be run simultaneously without undue interference and overlapping interest, for the most part.

In the late 60's and the early part of the 1970's, Raman spectroscopy experienced spectacular advances, mainly because of the new laser sources. The greater portion of the meeting at the University of Freiburg was concerned with molecular applications, and it was fairly clear that Raman spectroscopy was rapidly becoming a mature field and that no major breakthrough was predictable in the foreseeable future in the applications to vibrational assignments, molecular symmetry, and general bonding evaluations.

The major new technique concerned coherent anti-Stokes Raman scattering (CARS) and there were eight papers on this subject. It appears that this is a very powerful tool for the analysis of gases in reactive media and at very low concentrations. There are still some fairly formidable experimental difficulties remaining to be solved, but in general, it appears that CARS has great promise in the field of pollution and analytical applications.

In the new techniques area there was also a paper on the suppression of luminescence by FM Raman spectroscopy. The technique is relatively simple in concept, and the laser light incident on the sample is modulated in frequency between two closely spaced values, and the difference of the sample response at the two frequencies is recorded. The FM method automatically cancels out any contribution to the detector output which is independent of the laser frequency. The simplest way to contribute a multiplier dark count and stray room light. Additionally, luminescence peaks do not shift in the experiment and can, therefore, be made to cancel out. Related equipment was displayed in the exhibition hall along with other systems which utilized multichannel detection. Also in the new techniques area were papers on laser microscopy using the Raman effect, multichannel detection of Raman spectra, and a new micro-Raman spectrometer for particle analysis. The new laser Raman microprobe provides screen viewing of the microscopic Raman image of a sample radiated by a laser at a specific Raman frequency. The spectrum of a portion of the microscopic preparation can be recorded and by multichannel analysis of the spectrum, one can follow changes in microscopic images.

The one area which appears to be quite popular and showing considerable progress concerns the application of Raman spectroscopy to biomedical or biological problems. In the past there had been considerable difficulties in recording spectra of such systems and the amount of data obtained was fairly limited. However, during this meeting there appeared to be a large number of papers where solution of scientific problems had been solved and the earlier experience of sample handling was not as evident. The application of resonance Raman effect has enabled a large number of scientists to obtain spectra on complex biological systems, and this field appears to be one of the most productive at this time. Resonance Raman spectroscopy has been utilized in probes for drugs, immunology and enzyme reactions along with studies on nucleic acids and proteins. This is an extremely active area, and one would anticipate considerable scientific activity in this field for some time to come.

Finally, the organizing committee made up of Drs. Schmid, Brandmüller, Kiefer, Pantani, Schrader, and Schröter should be complimented on the excellent running of the conference. The overall organization was superb.

In conclusion, the conference was a highly successful scientific meeting, and everyone had an unforgettable stay in the city of Freiburg. Dr. James R. Durig of the University of South Carolina was appointed chairman of the Sixth International Raman Conference which will be held in Bangalore, India in 1978.