THE COBLENTZ SOCIETY

NEWSLETTER

Mailing No. 62 May 20, 1974

Report from Cleveland

Dr. J. R. Durig was elected President, and R. J. Jacobsen, Vice President of the Society. Newly elected members of the Board of Management are James Elliott and Peter Griffiths, replacing Kermit Whetsel and Robert Bauman.

From the Annual Meeting -

President's report (Dr. R. P. Bauman). The Society is now soundly in the black financially, and is able to proceed with its primary objective: to aid the practicing spectroscopist. For example, the Education Committee organized three instructional clinics at the 1974 Cleveland meeting, including a new introductory Raman Techniques session directed by B. J. Bulkin. An introductory infrared techniques clinic will be offered at the FACSS meeting in Atlantic City this fall. The spectrum publication program is proceeding well; 9000 reference spectra have been published, and work on Vol. 10 is underway. Dr. R. N. Jones' committee has updated specifications for Class II spectra to incorporate spectra taken with Fourier Transform spectrometers. On the less favorable side, membership has steadily declined, possibly because Society activities tend to support infrared spectroscopy in general rather than members in particular. There is also a general impression that the Society's focus of interest is inadequate to meet the broader needs of the practicing spectroscopist. The Board of Management is wrestling with these problems.

After discussion from the floor, the meeting was turned over to the new president, James R. Durig, who suggested the following goals for the next year:

Increase membership
Provide relevant service to members
Re-examine the Society objectives

From the Board of Managers meetings -

Howard Sloane and Paul Wilks were appointed to the Board of Managers for one-year terms to fill vacancies created by expansion of the board. A change in the By-Laws extending terms to four years has been approved.

Changes in the Newsletter were suggested, and an editorial committee was appointed.

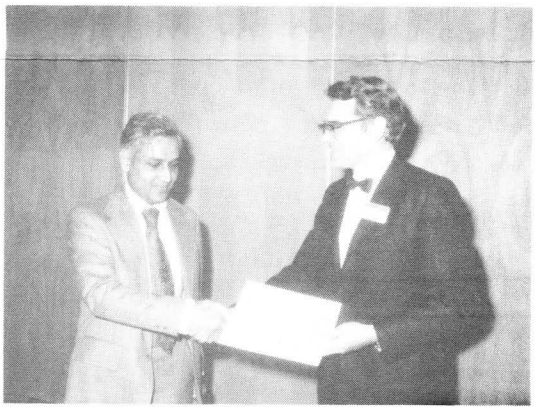
Needs for paid assistance in carrying out accounting, billing, IRS reports, etc., was discussed.

A number of suggestions for increasing service were discussed, including:

A speaker's bureau
Publication of a bibliography of specialized spectral data collection
Question and answer column for the Newsletter
Applications-oriented symposia at different scientific meetings
Publication of useful spectra not meeting Class III specifications
Establishment of a liaison group to interface with organizations such as OSHA
Introductory infrared clinic at FACSS and other scientific meetings

Committee Assignments

Cleveland Symposium	- James Elliott
Education	- Jeanette Grasselli, Dana Mayo, Robert Bauman
FACSS Liaison	- Jeanette Grasselli
Finance	- Robert Jakobsen
Joint Committee Liaison	- Lee Smith
Membership	- Ron Kagel, Freeman Bentley, Clara Craver, Bob Hannah
Newsletter	- Lee Smith, Paul Wilks
Spectrum Evaluation	- Norman Jones



Instructor J. S. Mattson (R) and students at the Introductory Infrared Techniques Clinic. Other faculty members included F. S. Parker, R. W. Hannah, R. J. Manning, and Jeanette G. Grasselli.

Treasurer's Report

Balance on hand February 16, 1973		$1,852.04
RECEIPTS:		
Dues	$ 601.00	
Sales of Spectra - Notebook edition	24,953.30	
Sales of Spectra - Microfilm	9,777.40	
IR Clinics	1,100.00	
Pittsburgh Conference Support	800.00	
	$37,231.70	
PAYMENTS:		
Operating expenses - Mailings, Pittsburgh Conference, Coblentz Symposium, misc.	1,697.67	
Coblentz Society reference spectra publication program	30,939.91	
	$32,637.58	
Balance on hand February 21, 1974		$6,446.16

Respectfully submitted,

Howard J. Sloane, Treasurer

Raman Techniques

Dr. Bernard J. Bulkin of Hunter College, N.Y. has prepared a 35-mm slide-tape course on Raman techniques. The material may be borrowed by Coblentz Society members without charge. Requests should be made to Mrs. Marcia Snaveley, The Standard Oil Co. (Ohio), 4440 Warrensville Center Road, Cleveland, Ohio 44128. Super-8-mm films on "Making a Mull" and "Optimizing the Spectrometer" are also available for loan from Mrs. Snaveley.

Silver Anniversaries

1949 must have been a good year for creative people, because a number of silver anniversaries are being celebrated in 1974. Of particular interest to spectroscopists are the Infrared Institutes of Fisk University and MIT. Fisk plans a special celebration during their session 12-16 August to recognize their quarter-century of service, and to look forward to the next 25 years. The institute, under the direction of Professor Nelson Fuson, includes concurrent sessions on Basic Infrared Spectroscopy and on Interpretation of Infrared and Raman Spectra. Former faculty members and students are invited to participate in the Silver Jubilee festivities on Friday, August 16.

The MIT Infrared Applications course, held in Cambridge for 22 years, is now given at Bowdoin College in Brunswick, Maine, August 5-9. The faculty includes Drs. L. J. Bellamy, E. R. Lippincott, Dana Mayo, and F. A. Miller.

Touring The Labs

Thumbnail Sketch of J. S. Mattson's Infrared Spectroscopy Laboratory at the University of Miami -

Our laboratory is located at the Rosenstiel School of Marine and Atmospheric Science, on the island of Virginia Key in Miami, Florida. The research interests of the students and staff of the lab vary from studies of the degradation of oil slicks to blood coagulation phenomena, the common denominator being infrared spectroscopy. The laboratory work revolves around a Perkin-Elmer 180, although other spectrometers, gas chromatographs, etc., are used in conjunction with several studies.

The 180 has been interfaced directly with an on-line minicomputer, a Data General Nova 1220. The on-line computer enables the spectroscopist to average spectra, perform real-time absorbance subtractions, mathematically smooth in real-time, and generally "massage" incoming data for instantaneous transmission back to the 180's flat-bed chart recorder. The computer system contains 16K of core memory, as well as an interface developed by the laboratory staff to handle the incoming and outgoing data. A three-drive cassette tape system is being added which will provide substantially more storage space for spectra and software.

Current applications of the computer-assisted spectrometer include: (1) A study of proteins adsorbed at the solid-aqueous solution interface, with germanium, and metal-coated germanium, in the internal reflection mode. The computer is used to remove the Ge metal-water baseline. (2) A study of long-term changes in the infrared spectra of crude oil slicks. (3) Corrosion studies. (4) An examination of adsorption mechanisms of naturally-occurring organics in sea water onto the surfaces of calcite and aragonite.

Q and A

This is a new feature of the Newsletter. If you have a question having to do with infrared spectroscopy--techniques, interpretation, or whatever--send it to

Q & A
The Coblentz Society, Inc.
P.O. Box 9952
Kirkwood, Missouri 63122

If you need an immediate answer, please enclose a self-stamped envelope. Otherwise, the answer (by a knowledgeable member of the infrared community) will be published in the next Newsletter with a request for response from the membership. It is hoped that many Coblentz Society members will participate, either by submitting questions or sharing their knowledge with a questioner.

Q: Are there any measurable changes in the polarization ratio of a globar as a function of aging?

A: We know of no studies on this topic, but would not expect any polarization effects from the rough, non-oriented globar surface. The spectrometer does, of course, polarize the radiation, and the degree of polarization changes with wavelength. This polarization ratio could conceivably change with time, but we would expect such changes to be small.

Q: Can anyone supply a foolproof method for "in-house" repolishing of worn KRS-5 internal reflection elements? Details, including the polishing cloth used, abrasive (if needed), solvent, etc., would certainly be welcome.

A: Because both the entrance and exit windows and the reflecting surfaces of the IRE must be optically flat, the repolishing problem is not a simple one. Also, thallium is very poisonous, so that inhalation of dust from grinding or absorption of dissolved KRS-5 through the skin or breaks in the skin can lead to severe problems. However, it is obvious that the polishing can be safely and effectively carried out by those properly equipped and trained. Can anyone offer any further comments?

Q: The table on page 141 of "Internal Reflection Spectroscopy," by N. J. Harrick, shows that diamond transmits from 0.25μm to >80μm. Partial transmission curves were made in the early 1950s at the University of Michigan and at Ohio State University, but little has appeared in the infrared spectroscopy literature. If anyone has some experience with diamond, either as a transmission cell or an internal reflection element, I would be interested in seeing some complete baseline spectra. It would also be helpful to know where one can purchase diamond windows or IREs, and what to expect in terms of size and cost.

A. Can anyone help? Please send your comments to the Q & A address given above.

What's Wrong With This Spectrum?

Problem in Mailing No. 60. Note that the sample is an amine hydrochloride, prepared as a KBr pellet. In many cases, partial halide exchange occurs during pressing, so the resulting spectrum may not be either that of the hydrochloride or hydrobromide, but an unpredictable mixture of the two. Such spectra are not reproducible; the safest sampling technique for amine hydrochlorides is the oil mull method.

Infrared Data for Occupational Health Studies

With the increasing emphasis on providing safe working atmospheres, infrared spectroscopists may be called upon more frequently to carry out low level vapor analyses. An infrared spectrometer equipped with a long path gas cell can generally supply spectral data permitting the qualitative indentification of most of the materials on the OSHA list when they are present in concentrations of about 10 ppm or more. Quantitative analyses can be made on considerably lower concentrations.

The instrument companies have published a number of reports and collections of vapor phase spectra that will be of direct assistance to spectroscipists working in this field. A list of the publications currently available is given below:

Available from Perkin-Elmer[1]:

IRB-14 - Infrared Determination of Detection Limits of Various Air Pollutants
IRB-36 - Reference Spectra of Gases
IRB-37 - Infrared Analysis of Toxic Vapors at the OSHA Concentration Limit
IRB-38 - Infrared Reference Spectra of Vapors at the OSHA Concentration Limit

Available from Wilks Scientific[2]:

OSHA Wall Chart incorporating toxic limits and infrared analytical data
AR-4 - Infrared Analysis of Vinyl Chloride at concentrations below 100 ppm
"Infrared Spectra of Gases and Vapors," Volume I - Prism Spectra (Erley and Blake, Dow Chemical Co.) Price $6
"Infrared Spectra of Gases and Vapors," Volume II - Grating Spectra (Erley and Blake, Dow Chemical Co.) Price $6

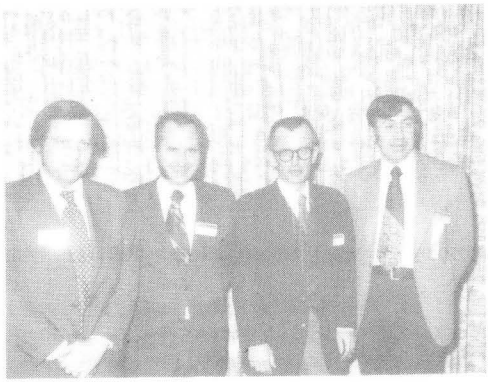
Available from Beckman[3]:

TR-590 - Infrared Spectra of Hazardous Gases and Vapors at OSHA Maximum Tolerance Levels - 62 Spectra. Price $5
TR-592 - Operating Characteristics of 20 meter cells
TR-595 - Infrared Spectra and Physical Constants of more than 200 OSHA Toxic Materials

[1]The Perkin-Elmer Corp. Inc.
761 Main Avenue
Norwalk, CT 06851

[2]Wilks Scientific Corp.
P.O. Box 449
S. Norwalk, CT 06856

[3]Beckman Instruments, Inc.
2500 Harbor Boulevard
Fullerton, CA 92634



Officers of the Coblentz Society line up for a mug shot. L to R Howard Sloan, Jim Durig, Bob Jakobsen, and Bob Hannah.

Seminar on Environmental Problems

Cosponsored by the Coblentz Society and the Ohio State University Symposium on Molecular Structure and Spectroscopy. Session TA, Tuesday, June 11, 9 a.m.

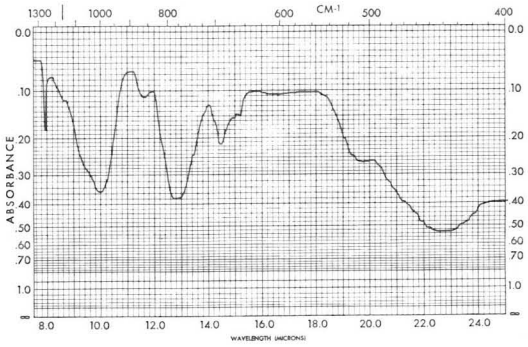
Opening Remarks
Allen S. Lefohn, U.S. Environmental Protection Agency, Corvallis, Oregon
Measurement Needs in Air Pollution: A Case for Spectroscopy
William H. Kirchhoff, National Bureau of Standards, Washington, D.C. 20234
Mechanistic Consideration of Chemical Reactions in the Urban Atmosphere
Jack Calvert, Department of Chemistry, The Ohio State University Columbus, Ohio 43210
Stratospheric Infrared Spectroscopy
Robert Toth, Space Science Division Jet Propulsion Laboratory Pasadena, California 91103
Spectroscopic Techniques
William F. Herget U.S. Environmental Protection Agency National Environmental Research Center Research Triangle Park, North Carolina 27711

This symposium was arranged by Bob Jacobsen in cooperation with Dr. K. N. Rao, Ohio State University Department of Physics.

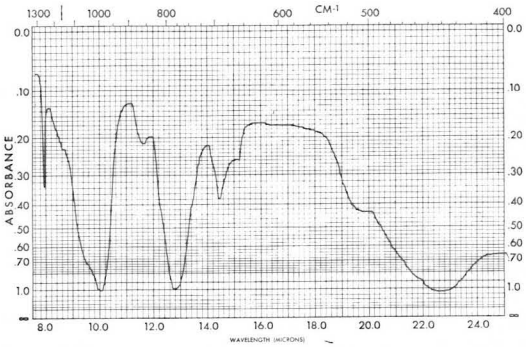
Using Infrared to Solve Real World Problems

What kind of rubber is in this O-ring?

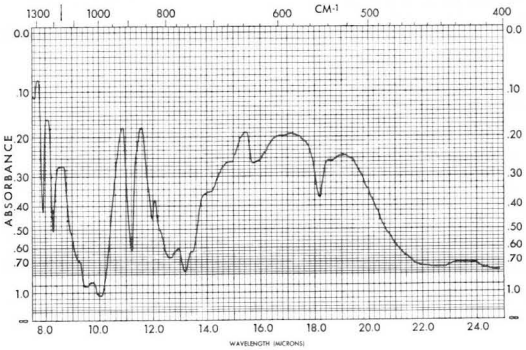
Several destructive tests might be used to solve this problem including burn-and-sniff, but non-destructive tests are more difficult and often less definitive. One of the best non-destructive methods is an infrared spectrum using a multiple internal reflectance (MIR) accessory. In this case, the O-ring was known to be a silicone, but it was not known whether the rubber was oil-resistant fluo silicone or conventional polydimethylsiloxane based. The MIR spectrum of the unknown clearly showed that it was a conventional material, and further, even indicated on which commercial composition it was based.
Analysis time: 10 minutes



MIR spectrum of conventional silicone rubber O-ring



MIR spectrum of unknown O-ring



MIR spectrum of fluorosilicone rubber O-ring

Contributions to this column are invited. Please send to the editor.

The Newsletter is published by the Coblentz Society, Inc. Editor is A. Lee Smith, Dow Corning Corporation, Midland, Michigan 48640. Comments and suggestions are invited.