THE COBLENTZ SOCIETY NEWSLETTER

Mailing No. 54 May 1, 1972

I. New Officers

Robert P. Bauman was elected President of the Coblentz Society at the March 7 Board of Managers' Meeting, replacing Jim Scherer, whose term of office expired. Howard Sloane was elected treasurer, replacing Bill Potts. Bob Hannah continues as Secretary of the Society.

Coblentz Award Winner George Leroi receives the award from President James R. Scherer.

II. Annual Meeting of the Coblentz Society (March 9, 1972)

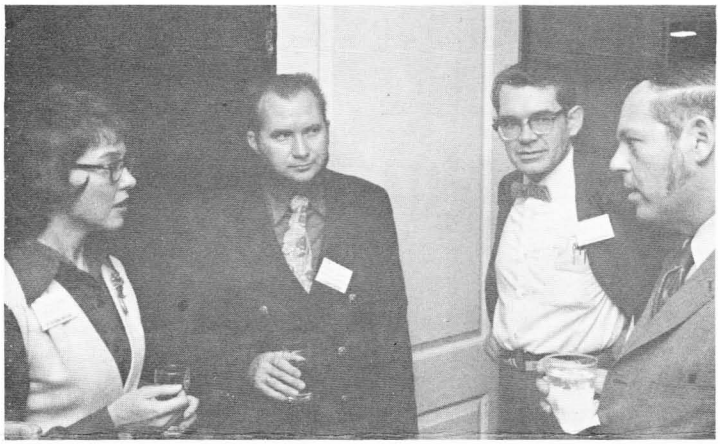
The meeting was called to order by President James Scherer at 5 p.m. in the Cleveland Convention Center Ballroom. The new officers were announced and the President thanked Bill Potts on behalf of the membership for his effort and time over the past several years. The President also noted the Coblentz Symposium, to be chaired by Prof. R. C. Lord, at the Ohio State Symposium on Friday, June 16.

Committee Reports Were Given

A. Membership; R. P. Bauman and R. W. Hannah. Membership is currently 680. A membership drive will be conducted this year.

B. Raman; E. Becker, R. Kagel, I. Levin. A new Raman Technical Group has been formed (Ellis Lippincott, Chairman) and has affiliated with the Optical Society of America. This group will sponsor symposia at OSA meetings, and is responsible for publication of the Raman Newsletter. The following recommendation for the Coblentz Society were presented: Continued recognition by the Society of the complementary nature of IR and Raman spectroscopy, and emphasis on the uses of Raman through symposia, etc.; dissemination of information on uses of Raman spectroscopy and recommendations for the presentation of spectra; education of programs such as workshops and filmstrips; and generation of a limited number of high quality Raman spectra for inclusion in the Class II infrared compilation now being prepared.

C. Education - J. Grasselli - The Advanced Infrared Techniques Clinic scheduled for Friday, March 10 has 11 registrants. The Education Committee plans to arrange for additional programs, some at a more elementary level.



Jeanette Grasselli, Jim Durig, Bob Bauman, and Howard Sloane get an early start on business at the Board of Managers' dinner meeting.

D. Evaluation of Reference Spectra - R. N. Jones. Class II specifications are being modified to cover both Fourier Transform and dispersive spectrometers.

E. Coblentz Spectra Publication - C. D. Craver. A $10,000 grant from the Office of Standard Reference Data is being used to support assembly of a small (100 spectra) coherent set of Class II infrared spectra. These spectra will be used to test and demonstrate the advantages of high quality spectra. Set 8 of the standard Coblentz Spectra is now available from Sadtler Laboratories. Work on Set 9 will be deferred in favor of the Class II spectra program supported by the OSRD.

F. 1973 Pittsburgh Symposium - J. Durig (K. Whetsel). A list of possible subjects was generated by attendees and will be voted on by the membership.

The new President, Dr. R. P. Bauman, then reviewed the purpose and activities of the Coblentz Society. The Society:

Provides a forum for expression of needs of the spectroscopic community in infrared and Raman spectroscopy;

Gives encouragement to workers in the field (e.g., the Coblentz Award);

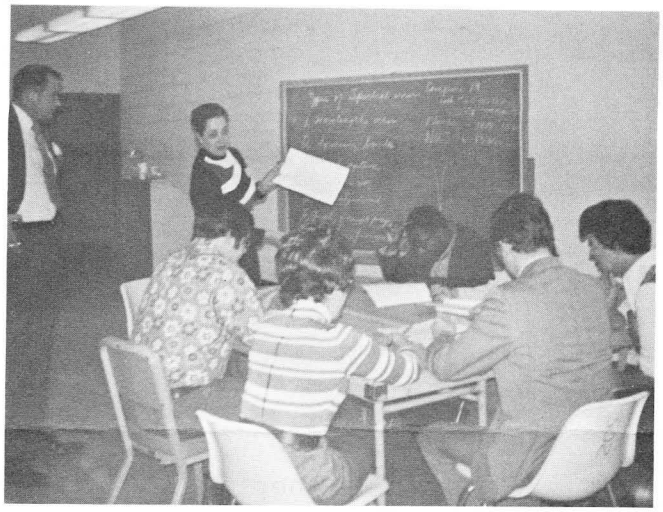
Organizes symposia on current topics of wide interest;

Develops educational programs;

Fills unmet needs in the field.

He noted that the Society does not exist to do things for its members. It exists to help the members do things for themselves.

The meeting was adjourned at 6 p.m.



Clara Craver discusses a problem spectrum at the Advanced Infrared Techniques Clinic as Bill Potts looks on.

III. Board of Managers' Meeting (March 7, 1972)

In addition to topics already reported under item II, the following were discussed.

A. Coblentz Award. The scope of consideration for the work of the Coblentz Awardee was changed from "infrared spectroscopy" to "molecular spectroscopy."

B. Coblentz Spectra. Board approval was given for Mrs. Clara Craver to submit a proposal to OSRD seeking $20,000 for support of the Class II spectra program, the emphasis to be on well-defined classes of compounds.

There was a significant and prolonged discussion relating to the Coblentz spectra collection. The problems are:

1. Sales income has not kept pace with expenses, although sales of Set 6 are now approaching the break-even point.

2. The publisher is not meeting his contractual obligations as to publication schedules, royalty payments, or sales reports.

3. Should the Society be in the business of producing spectra collections, since good quality collections are now available commercially? Should Class II spectra be a larger part of the effort, or perhaps the entire effort?

The Board voted to institute an ad hoc committee to recommend a policy for the spectra publication program.

C. Finance. The Finance Committee was directed to consider alternative plans for dealing with the spectra publication program and make a recommendation to the Board of Management. Options include finding another printer; issuing smaller groups of spectra; or selling the collection to a commercial publisher.

IV. Treasurer's Report (March 6, 1972)

Balance on hand March 2, 1971		$345.53
Receipts:		
Dues	$ 1,137.19	
Royalty payments - Sadtler	10,937.25	
NBS support of programs	2,500.00	
Microfilm sales	2,363.00	
Miscellaneous	150.00	
	$17,087.44	
Payments:		
Operating expenses: mailing postage, stationery, misc.	$ 1,267.94	
Spectra preparation program	13,864.90	
Class II Spectra program	2,078.08	
	$17,210.92	
Balance on hand March 6, 1972		$222.05

Respectfully submitted,

W. J. Potts, Treasurer

V. Coblentz Society-Sponsored Symposium at Columbus
Friday, June 16, 1972 - 9:00 a.m.

HIGH RESOLUTION NMR SPECTROSCOPY OF BIOLOGICAL MATERIALS
W. D. Phillips, E. I. duPont de Nemours and Company

RESONANCE RAMAN SPECTROSCOPY OF SOME HIGHER CONJUGATED BIOLOGICAL MATERIALS
L. Rimai, Ford Motor Company

INTERMOLECULAR COUPLING IN THE VIBRATIONAL SPECTRA OF BETA-POLYPEPTIDES
S. Krimm, University of Michigan

RAMAN SPECTROSCOPIC STUDIES OF CONFORMATIONAL CHANGES IN PROTEIN DENATURATION
R. C. Lord, Massachusetts Institute of Technology

INFRARED SPECTROSCOPY OF METAL PROTEINS
James O. Alben, The Ohio State University

VI. Advanced Infrared Techniques Clinic

Another successful Advanced Infrared Techniques Clinic, sponsored by the Coblentz Society, was held on Friday, March 10, during the Pittsburgh Conference in Cleveland, Ohio. The purpose of the clinic is to provide a workshop experience for an advanced spectroscopist to optimize his techniques for obtaining high quality (Class II) infrared spectra and to sharpen his critical eye for general evaluation of spectra. Eleven students, under the direction of a faculty of five, spent the day actually preparing a Class II Nujol mull, operating instruments to record a Class II spectrum, and analyzing problem spectra. Two short movies produced by the Coblentz Society were shown on "how to prepare a mull" and "how to operate a spectrometer." The staff consisted of:

W. J. Potts, Jr., Dow Chemical Company;
R. N. Jones, National Research Council of Canada;
C. D. Craver, Chemir Laboratories;
R. W. Hannah, Perkin-Elmer; and
P. Taimsalu, Beckman Instruments.

VII. Spectrum Publication Questionnaire

The Board of Management of the Coblentz Society needs to determine the feelings of the membership to assist them in establishing policy in present and future Coblentz-sponsored programs. We ask that you express your opinions by completing and returning the enclosed questionnaire. In order to minimize your effort and gain information on certain specific questions, the questionnaire is in multiple choice format. However, we invite you to elaborate on any of the items.

BACKGROUND ON INFRARED SPECTRAL PUBLICATION PROGRAM

The spectral publication program of the Coblentz Society had its origin in discussion meetings at the OSU spectroscopy conference in the mid-1950's. Subsequently, a questionnaire mailed to all members confirmed a general need for more and better reference spectra. Policies and goals were worked out by an infrared committee and were approved by the Board of Managers.

The scope of the project and/or method of operation decided upon were:

Coblentz spectra should be of higher quality or add data to already published spectra of any given compound. If the spectrum of a compound was not already available in the literature, a spectrum approved for the Coblentz Society catalog needed to be consistent with the structure and of sufficient quality to be "useful" for compound identification.

Since there was no funding available, the first set of 1,000 spectra was prepared as a voluntary committee effort for the Society, and Sadtler Laboratories agreed to bear the initial printing and marketing costs in return for royalty payments on sales.

The committee members realized that a fully volunteer effort would be too burdensome to continue indefinitely. To pay for the spectral collection, evaluation, and editing a budget was based on a spectral sales price which would yield the Society $5,000 per volume published, at a sales level of 100 sets. This $5 per spectrum was to be used to prepare future volumes.

Five thousand spectra were prepared in this fashion, and have been a useful and profitable effort.

The direction of this program changed significantly in the mid-1960's. At the request of the Office of Standard Reference Data of the National Bureau of Standards, the Board of Managers established criteria for Research Quality and Analytical Quality spectra. It then began using these specifications in Volumes 6, 7, and 8 under the combined auspices of the National Standard Reference Data System and the Joint Committee on Atomic and Molecular Physical Data.

It was evident that preparation of spectra for this higher quality publication would be more expensive. Four spectra were being collected and evaluated for each spectrum approved for publication; formal nomenclature was required; draftsman quality structure labels were to be prepared; spectra were to be photographically reduced to nearly uniform size.

The Board of Managers approved a processing cost of up to $25 per published spectrum, and increased the sales price of the spectra in anticipation of a break-even point at 180 to 200 customers.

At this time, Set 6 has sold 140 sets, Set 7 about 90 sets, and Set 8 has just become available. Thus the Society has assets in volumes of spectra for sale, but it is showing a cash-flow deficit. Over the past three years, this deficit has varied from about $20,000 when a newly prepared volume has not yet been shipped, to about $11,000 when major sales have occurred for a new volume and there has not been much effort expended toward a new set.

It is projected that it will be at least another year before Set 6 costs are fully recovered. It can be reasonably projected that most buyers of Set 6 will also purchase Sets 7 and 8, and that these volumes will return their initial cost somewhat quicker than has been realized for Set 6.