I. Election of Officers

At the Board of Managers meeting in Cleveland on March 4, 1969, Dr. Charles Angell was unanimously elected President of the Society. R. W. Hannah was reelected Secretary and W. J. Potts, Treasurer. The secretary reports that the newly elected members of the Board of Management are Dr. E. D. Becker and Dr. James R. Scherer.

II. Coblentz Society Symposium at Cleveland

Once again, the Coblentz Society-sponsored symposium at the Pittsburgh Conference was highly successful. Co-organizers Jeanette Grasselli and Ron Kagarise deserve a vote of thanks for their efforts.

Symposium speakers were (1 to r) R. S. McDonald, R. O. Crisler, J. G. Karohl, and Coblentz Award Winner, Dr. Giuseppi Zarbi.

III. General Membership Meeting

The annual discussion meeting was held Thursday, March 5 in the Whitehall Room of the Sheraton-Cleveland Hotel.

President Freeman Bentley welcomed the two new Board members, Drs. E. D. Becker and J. R. Scherer. He extended his thanks to the Board and the membership for their assistance during the past year. He also expressed appreciation to James Hamilton and Sadler Research Laboratories for sending the Coblentz brochure to Sadler customers. This mailing resulted
in about 100 new members. President Bentley noted that this was the 20th anniversary for the Fisk and MIT summer infrared institutes and congratulated the staffs of these two courses on their continued contribution to IR spectroscopy.

Committee reports were given as follows:

1. C. Angell, Membership. About 200 names were removed from the mailing list for failure to pay dues after several reminders. Approximately 70 new members joined the Society in 1968 and about 100 more since January 1, 1969.

2. R. N. Jones, Evaluation of Reference Spectra. It was suggested that descriptive names be used to describe the different classes of IR spectra: Critically Defined Physical Data (Class I), Research Quality Analytical Spectra (Class II), Approved Analytical Spectra (Class III). Dr. Jones also reviewed the function and plans of CODATA.

3. J. Grasselli, Infrared Techniques.

The study committee met at the Pittsburgh Conference and presented a progress report at the General Discussion Meeting of the Coblentz Society. The members of the advisory committee are Ted Hermann, Henry Morgan, Dick Nyquist, Conrad Phillippi, Howard Sloane, Edward Truschke, Paul Wilks and Lynn Wolfram. When the committee was established in September, the Coblentz Board suggested that an effective medium for disseminating instruction on good infrared technique would be movies. As a consequence a brief color 8 mm film on preparation of mulls was produced and directed by A. Lee Smith and W. J. Potts, Jr. and shown to the membership at the Discussion Meeting. The movie was very well received by those present, and it was generally agreed that such movies would be saleable to industry and Universities and constitute a worthy project for the Coblentz Society. Constructive advice given included a suggestion to either insert more explanatory written material into the film or supply a pamphlet with the film which would essentially serve as the narrative.

These suggestions will be acted upon by the committee. They, in addition, are considering a corollary pamphlet or brochure which would present clear, illustrated instructions on how to obtain spectral data from a given sample, with discussion on effect of various techniques on instrument performance and on data.
Pertinent reprints of literature articles, lists of commercial sources of materials, and a complete bibliography per technique would be included.

The subjects to be covered are mulls, pellets, liquids (neat, solution), micro methods, films (cast, pressed), compensated spectra, GC-IR, reflectance spectroscopy (specular, diffuse), pyrolysis, high and low temperature work.

Immediate plans are to complete the mull film "package" and get a cost estimate on materials and reproduction so that a decision can be made on offering this first project for sale. Drs. Smith and Potts have also agreed to prepare a second film demonstrating the proper way to set up and operate an infrared spectrometer.

4. C. Smith, Spectral Evaluation and Publication. Support is needed for this program, both donations of spectra and purchase of published compilations. Arrangements have been made with Applied Spectroscopy and with Analytical Chemistry for the Coblentz Society to publish compilations of spectra submitted by authors, provided minimum criteria are met.

More people are needed for evaluation. This is a paid service. Those who are competent in the interpretation of spectra for special classes of chemical compounds and who would like to participate are asked to contact Mrs. Clara D. Smith, Box 152, RD 2, Cranbury, New Jersey, 08512 for further information.

5. Discussion of possible 1970 Symposium topics was led by W. J. Potts. Results were: Laser Raman Spectroscopy - 25 votes; Computer handling of structural data - 0; Pseudo-matrix isolation - 1; Chemical bonding - 5.

Chairman of the 1970 Symposium is J. Scherer.

6. Committee Appointments

a. Treasury Audit: E. D. Becker, J. Scherer
b. 1970 Symposium: J. Scherer
c. 1970 Pittsburgh Conf. liaison: W. Fateley, J. Grasselli
d. N.B.S. contract: C. Angell
e. Membership and Publicity: E. D. Becker, R. W. Hannah
- 4 -

f. IR Techniques: J. Grasselli
g. By-laws: To be appointed by the president
h. Nominations: to be appointed by the president
i. Liaison with SAS: J. Grasselli

IV. Board of Managers Meeting at Cleveland

A. Spectral Publication Program (Clara Smith)

Up to the present, the spectral publication program has been carried out at a preparation cost of $5,000 per set of 1000 spectra. This money was recovered by sales of 100 sets; on sales of over 100 sets, the Society made a profit of $30 per set. Since joining the Joint Committee program (see below), the Society is still investing $5,000 per set of 1000 spectra. Preparation now includes evaluation and a more business-like and informative format, so costs are higher and the sales price has been increased. Also, the break-even point is now 150 sets.

It has also been necessary to move from one set to the next without waiting for income from earlier sets. Set 6 is now ready and will be available soon; set 7 has 350 evaluated spectra and hopefully, will be published in the fall. However, money must be found to support this interim processing effort. The initial spectra collection activities were supported by the NSRDS; these funds have now been exhausted.

A discussion then followed concerned with possible sources of money for support. Some suggestions were made which will be investigated further.

B. Joint Committee on Atomic and Molecular Physical Data (A. Lee Smith)

The objective of the Joint Committee is to promote distribution of evaluated physical data. Initial efforts have been concentrated on infrared spectra; other fields such as NMR, Raman, mass and electron spectroscopy will be looked at to determine if a need for evaluated data exists.

Two sets of contracted Class II infrared spectra have been received. Careful inspection of these spectra suggests that further education on techniques of sample preparation and of running an infrared spectrometer is needed. A one-half day clinic on Advanced Infrared
Techniques for production of Class II spectra was suggested for the 1970 Pittsburgh Conference. R. N. Jones and A. L. Smith were appointed to chair a committee to consider this suggestion and make a recommendation to the Board.

C. Other topics discussed are covered elsewhere in this Newsletter.

V. Dues Reminder

Those members who have not yet paid their 1969 dues are requested to do so as soon as possible. Dues are $2.00 per year or $5.00 for three years.

VI. Meeting at Mid-America Symposium

All infrared spectroscopists are invited to a discussion meeting on Reference Spectra and Retrieval Systems to be held May 14 at 2:00 p.m. in the Caracas Room of the Sheraton-Chicago Hotel. This is an information symposium to acquaint conferees with the activities of scientific organizations in the field of reference spectra, principally infrared absorption spectra. Short talks will be presented by representatives of four of the active organizations and audience contributions and questions are encouraged.

DISCUSSION MEETING ON REFERENCE SPECTRA AND RETRIEVAL SYSTEMS

Chairman: Clara D. Smith

(1) The Role of the National Standard Reference Data System in Spectral Data Collection.

The National Bureau of Standards Office of Standard Reference Data has embarked on a program of encouraging the collection and dissemination of a carefully measured and well evaluated spectra. As a first step it had the Coblentz Society prepare a document listing the necessary criteria for assessing the quality of infrared spectra. In conjunction with the Joint Committee for Atomic and Molecular Physical Data, it has sponsored the issuance of a new series of evaluated NSRDS-Coblentz Society Infrared spectra. The first set of 1000 spectra will soon be published. It now hopes to extend these activities to aid in the upgrading of Raman, NMR and other types of spectra where the criteria for acceptable spectra are not yet well defined. The
ultimate aim of this effort is to produce a body of
spectral data in all the abovementioned areas which
will serve as a source of high quality reference
information.

(2) Collection and Evaluation of Infrared Spectra in the
Coblentz Society Catalog.
Clara D. Smith, Infrared Consultant, Chemir Laboratories,
R. D. 2, Cranbury, New Jersey 08512.

The purpose and history of the Coblentz Society program
will be briefly reviewed and spectra collected from
different sources will be used to demonstrate the new
evaluation criteria.

The cooperative program with Analytical Chemistry and
Applied Spectroscopy journals for publication of
spectra pertaining to research publications will be
described.

(3) The ASTM Infrared Data System - Present and Future.
R. M. Sherwood, American Society for Testing and

A brief account is given of the present status of the
data file with respect to collections included, book
indexes, and format in which spectral data are presented.
Retrieval of data by the ASTM-Dow search system is
illustrated and plans for a search service and time-
sharing are discussed.

(4) Class II Infrared Spectra: What, why, how?
A. Lee Smith, Dow Corning Corp., Midland, Michigan.

The following points will be considered:
* The need for Research Quality Analytical (Class II)
  Spectra.
* The experience of several laboratories trying to
  meet Class II standards.
* Instrumental and technique problems of producing
  Class II spectra and how to overcome them.
VII. What's Wrong with this Spectrum?

Newsletter is starting a new feature to test your diagnostic abilities. The spectrum (of indene) shown below was run on a modern grating spectrometer but with one or more of the parameters (slit, response, scan time, gain, etc.) incorrectly set. We can't offer an expense-paid vacation to Bermuda for the best answer, but we can publish it; so if you think you know what's wrong, drop a line to the editor, A. Lee Smith, Dow Corning Corporation, Midland, Michigan 48640.
Balance on hand March 1, 1968 $10,831.78

Receipts:

Dues $1,483.35
Sale of Coblenz Reprints 10.50
Royalties from Sadtler1 290.00
Sale of Microfilm 1,195.50
Travel, NSRDS contract2 1,798.25
$4,777.60

Disbursements:

Operating expenses (secretarial, postage, mailings, stationery, misc.) $2,067.91
Publicity 162.58
Coblenz Award; travel and prize 205.00
Coblenz Symposium Speaker 216.00
Travel, NSRDS contract2 1,798.25
Large-letter typewriter 319.30
Spectral Publication expense3 6,342.99
$11,112.03

Balance on hand March 1, 19694 $4,497.35

Respectfully submitted,

W. J. Potts, Treasurer

Notes

1 To May, 1968.

2 The NSRDS contract (specifications for reference spectra) has been completed. Some travel funds remain; these are being used for special meetings concerned with current evaluation problems.

3 Includes processing of some spectra for Set No. 7.

4 On September 18, 1968, $3,000 were invested in six month Certificates of Deposit paying 5%, and $1,000 was placed in a savings account.
EVALUATED INFRARED SPECTRA

Collected by The Joint Committee on Atomic and Molecular Physical Data

Published by The Coblentz Society, Inc.

The Coblentz Society is proud to announce the availability of 1000 high quality infrared spectra. Although technically a continuation of the Coblentz Spectra series, the spectra have been evaluated by expert spectroscopists and selected to meet criteria established by the Coblentz Society for the National Standard Reference Data Program. Included in the current issue are 500 pharmaceuticals, 100 organosilicon compounds, and 400 general organic structures.

These spectra have been contributed by various infrared laboratories, and each must meet the following criteria to be included:

1. It is a better quality spectrum than any previously published for this compound, or is a spectrum not previously published, and

2. Each spectrum has been critically evaluated by competent spectroscopists as to its technical quality (must meet or exceed the criteria for Class III reference spectra, as established by Coblentz Society (Anal. Chem. 38, No. 9, p. 27A), and its consistency with the assigned chemical structure).

It is planned to issue these spectra in blocks of 1000. The first 1000 spectra are now ready for publication, and will be available by early Summer 1969. They may be ordered from Sadtler Research Laboratories, 3316 Spring Garden Street, Philadelphia, Pennsylvania 19104, who are serving as publishers.

Price: $265.00/1000 spectra, including loose-leaf binders.

Specifications: Printed one spectrum to a page including approved chemical name, structural and molecular formula, state, melting or boiling point, and notation as to how the spectrum was obtained. A sample spectrum appears on the reverse side of this sheet.
3,4-Dimethoxyphenylacetic acid

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NSRDS - COBLENTZ CLASS III

Structure Verified

State: Solid
M.P.: B.P.

Contribution Lab:
The Dow Chemical Company

Date Recorded: 6.4.68