THE COBLENTZ SOCIETY

MAILING NO. 5 October 1, 1957

Minutes of The Coblentz Society Discussion Meeting at Ohio State University Symposium held on June 11, 1957.

1. New Officers - It was announced that the new members of the Executive Board elected by the membership are R. C. Lord, Director, Spectroscopy Laboratory, Massachusetts Institute of Technology, Cambridge 39, Massachusetts; and Foil A. Miller, Mellon Institute, Pittsburgh 13, Pennsylvania, replacing Howard Cary and Bryce Crawford. The present Executive Board consists of:

Drs: E. J. Rosenbaum
     E. D. McAllister
     N. Wright
     F. A. Miller
     H. H. Nielsen
     R. C. Lord
     V. Z. Williams

Subsequent to the election, Foil Miller accepted an opportunity to spend a year abroad. Dr. R. A. Friedel is acting for Dr. Miller during this period.

2. Norman Wright reviewed the intent and purpose of the Coblentz Society as presented in the Coblentz Society Mailing No. 4, April 10, 1957.

3. Dr. Marion Kranc of Pittsburgh Coke and Chemical Company reported on his initial attempts to start a local section of the Coblentz Society in the Pittsburgh area. Thirty names were available from the Mailing List and of this list, sixteen expressed interest in such a possibility. This resulted in a general discussion of the value of local sections.

It was felt that there would be value in such sections for the informal benefits that might be derived. For example; the local members could register their general infrared activity stating type of work done, instrument equipment, available spectra, area of compound handling to indicate possibility of pure materials, etc. Anyone in the membership facing a new problem could, by consulting this list, determine who in the area might be best able to help him. The group could also have periodic informal meetings for discussion of their mutual problems.

Dr. Crisler reported on Dr. Rosen's efforts to start a section in the Cincinnati area. They had discussed the problem with ACS and got their blessing, but not the desired result of the loan of a meeting place. The Cincinnati people intend to go ahead to set up informal discussion meetings.

4. Norman Wright reported on the status of the analytical methods collected by R. C. Wilkerson. There are now 36-40 submissions which were judged to be sufficient for sending to ANALYTICAL CHEMISTRY to get the program started.
4 - (contd.)

The attainment of this point in the program is certainly a fine accomplishment, but it has taken much longer than was expected in view of the initial membership response to this project. It is hoped that with the commitment of the program to ANALYTICAL CHEMISTRY, the membership will face the responsibility they have assumed and start working on the program rather than leaving the work to two or three member sites that have made the contribution so far.

5. Mrs. Clara D. Smith, of Battelle Memorial Institute, reported on the results of her survey of the membership to determine the status, membership reaction, and program with regard to infrared spectra availability. This report, the proposed program, and the subsequent action, are covered in Exhibit A and A-1.

Mrs. Smith's report brought out considerable discussion of the situation resulting in three basic group reactions that the main desire of the membership is to have more spectra available, to have better quality spectra available, and to get going on a program to accomplish these ends. The enclosed program, it is felt, is in accordance with this membership requirement and criticism or suggestions concerning it should be sent directly to Mrs. Clara D. Smith, Battelle Memorial Institute, 505 King Avenue, Columbus 1, Ohio.

The following comments are pertinent as of the date of this mailing:

1. There will be a Discussion Meeting at Pittsburgh in March 1958 and an agenda for discussion will be mailed before that time.

2. The proposal made by the Spectral Data Systems Committee as stated in Exhibit A-1 has been approved by the Executive Board and the Committee has been authorized to proceed.

3. There is enclosed, a statement of the Infrared Analytical Data Program present status. (Exhibit B)
This report is divided into two sections: A. Principal conclusions from the questionnaire returns, and B. Detailed answers to questions asked. The detailed answers are included where practical for permanent reference by members who may be interested in facets of the information not summarized by the committee.

Replies were received from at least 164 members. 36 returns did not specify number of members represented and were counted at the minimum of one member each.

A. Principal Conclusions Drawn by the Committee
From the Questionnaire Returns

There is a membership majority preference for having one central reference spectrum system, but this is far from being unanimous. 64 members favored support of only one system by the Coblentz Society as compared to 62 who favored support of all existing systems. Several of this 62 (not tabulated for an exact count) expressed the view that a single system was a desirable goal, but that the Coblentz Society as a unit should not operate to the detriment of any existing system. There was also a repeated comment that with reference spectra being so badly needed, duplication was a lesser evil than low output.

There is no agreement among members on which single system should be supported. The numerical results on this subject are:

<table>
<thead>
<tr>
<th>System</th>
<th>Members</th>
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<tbody>
<tr>
<td>API</td>
<td>21</td>
</tr>
<tr>
<td>NRC-NBS</td>
<td>21</td>
</tr>
<tr>
<td>Sadtler</td>
<td>12</td>
</tr>
<tr>
<td>DMS</td>
<td>20</td>
</tr>
</tbody>
</table>

There is a similarly divided interest among the membership on sorting systems. Users of IBM cards total 68, and of Keysort cards total 61. 37 members reported using both sorting systems and 32 use neither one. Although many users of IBM cards were vehement in denouncing Keysort systems, there are apparently a lot of members whose needs are served by Keysort decks on limited compound types, or who find that with proper pre-sorting of decks, the Keysort operation is desirable for them. The members who stated that they had a system but didn't use it were not included in these totals.

A frequently voiced opinion about the ASTM-IBM deck was that its value would be greatly enhanced if copies of the abstracted literature spectra were available with the deck.
Only three members expressed doubt about the merit of the Coblentz Society's assisting in getting reference spectra published. The large interest in getting more spectra available for public distribution is shown in part by the offers of contributions. 138 members (82 per cent) offered to contribute reference spectra. The total specifically offered is more than 17,000 spectra. On the assumption that duplication and failure to contribute might eliminate 2 out of 3 of the promised spectra, it still appears that as many as 5,000 reference spectra may be available for immediate publication if a suitable mechanism were in existence.

B. Summary of Results From Questionnaire on Existing Infrared Spectral Data Systems to Coblentz Society Members

Reported as number of members unless otherwise indicated.

I. Infrared Reference Spectra

A. Type of work done by your laboratory.

- 33 1. Control
- 101 2. Applied Chemical Spectroscopy
- 134 3. Research and development

(If more than one of these functions is performed by the laboratory, specify the one(s) for which use is made of published data.)

B. Spectral data available.

- 127 1. API
- 104 2. NRC - NBS
- 53 3. Sadtler
- 34 4. DMS
- 55 5. Other. Specify: Principally literature and own reference file

C. Spectral data most frequently used or otherwise considered most valuable. Rate all you use 1st, 2nd, 3rd, etc.

Tabulated as number of 1st place answers received. Many people, of course, inserted the added comment that their own file was most valuable to them.
D. What do you consider the major advantage and fault of each of the systems you use?

Most frequent comments:

1. API
   Advantage - purity of compounds; reliability
   Disadvantages - indexing system, folded wavelength scale, limited variety, too few.

2. NRC - NBS
   Principal comment - too few; Compound "series" helpful; quality variable.

3. Sadtler
   Advantage - large number, good reproduction, convenient form. Disadvantage - Spectrum quality and unreliability of compound purity.

4. DMS
   Most users withheld comments because of limited experience. Most frequent criticisms were on lack of sturdiness of paper stock used and smallness of spectrum. Praise of its "vigor" and "potentialities" was voiced.

E. Do you plan to purchase any of these catalogues?

(Replies counted by laboratory rather than by members.)

<table>
<thead>
<tr>
<th></th>
<th>Within Year</th>
<th>Future</th>
</tr>
</thead>
<tbody>
<tr>
<td>API</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>NRC-NBS</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>Sadtler</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>DMS</td>
<td>16</td>
<td>8</td>
</tr>
</tbody>
</table>
F. If you do not have, or plan to purchase one of these systems, why not? Please answer for each one that you do not buy.

No outstanding answer: "no need", "too expensive", "too limited", "too big", "has edge punch", "no edge punch", "card awkward", "sheet awkward", "too little".

G. If the Coblentz Society were to assist in these programs, do you favor support of

- 61 1. One system
- 21 API
- 21 NRC - NBS
- 12 Sadtler
- 20 DMS

- 62 2. Collection of spectra and distribution to all systems.


H. If the Coblentz Society were to assist in these programs, what would your laboratory do in the next year?

Contribute reference spectra? 138

How many? 17,000+

Contribute pure compounds? 13 laboratories

How many? 132 listed; mostly left a "?".

Contribute funds to support collection and selection of spectra? 10 laboratories

How much? Generally left dependent on system agreed upon.

II. Sorting Techniques - By laboratory

A. Do you have IRε equipment?

- 34 1. In your laboratory
- 58 2. Available at other locations
- 32 3. None available
B. Type IBM equipment available
   79  1. Sorter
   40  2. Collator

C. Do you use edge-punched cards?
   22  1. DMS
   45  2. NRC-NES
   8   3. Other. Specify: Own

D. Do you use IBM Cards?
   55  1. ASTM
   13  2. Other. Specify: Own

E. Do you plan to obtain IBM equipment?
   7   Within year
   15  Future

F. Do you plan to purchase ASTM-IBM index cards?
   9   Within year
   18  Future

III. Comments

Please state whether you are replying for one or more installations, or for more than one Coblenetz member in your lab. Any additional suggestions will be welcomed by the committee.

125 replies representing 184+ members.
PROPOSAL FOR A SPECTRUM COLLECTION SYSTEM

At the Coblentz Society Meeting at the Ohio State University in June, 1957, the committee on spectral data reported on returns from the membership questionnaire. One outstanding interest by the members seemed to be in obtaining a greater rate of spectrum publication. The committee proposed a course of action designed to give maximum opportunity for individual laboratories to contribute to existing spectral catalogues. This proposal, as approved by the members in attendance, is as follows:

1) The committee will appoint regional collectors, about 10 men, to collect and edit 100+ spectra each.

2) These spectra may be published with credit, or anonymously, as the contributing laboratory desires. Direct traces of original curves will be satisfactory if approved by the collector.

3) The collector will choose spectra to avoid duplication of existing files unless a new spectrum is an improvement over data already available. The criteria for selection will be quality and utility with no emphasis on uniformity of format.

4) This collection of 1000+ spectra will be forwarded to the committee for additional cross-comparison.

5) A resulting deck of 1000 spectra will be made available to current publishers of spectra under terms to be agreed upon, but with the following as major stipulations:

   a) The spectra will be published within a given time (e.g., 4 to 6 months).

   b) The spectra will be duplicated by a direct process to a scale no smaller than 1 cm./micron.

   c) The published Coblentz Donor Spectra may be purchased from the publisher as a block and separate from the rest of his available spectra. This is to permit individual users to purchase these spectra in the system he finds most useful without duplicating their purchase in all decks he buys.

6) If this system operates successfully, a share of the proceeds from the sale of the spectra should revert to the Coblentz Society for perpetuation of the collection on a non-volunteer basis.

If this proposal is approved, a first step will be a discussion with the possible publishers as to such financial reversion to the Society.

Clara D. Smith, Chairman
Coblentz Committee on Infrared Absorption Spectra
EXHIBIT B

STATUS OF INFRARED ANALYTICAL DATA

The Executive Board of the Coblentz Society is happy to state that the first series of Infrared Analytical Data will appear in the October 1957 issue of ANALYTICAL CHEMISTRY. This is one of the first programs to be initiated by the Coblentz Society and Society appreciation is certainly due the Review Committee under R. C. Wilkerson and the data submitters for the start that has been made.

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The Executive Board of the Coblentz Society is most unhappy to state that, unless the rate of data submission by the membership is increased, these publications cannot be continued. At the moment, there is a backlog of one and one-half issues. It is requested that each member who promised support so enthusiastically when the original survey was made in 1955, as well as new members, take time to read the ANALYTICAL CHEMISTRY article and look at the data with one question in mind -- 'Is the intent of this program, the broad availability of such data, of value to the field in which I am working?' If the answer is 'yes,' do something about it! If the answer is 'no,' it will be evident in a month or so.