THE COBLENTZ SOCIETY

NEWSLETTER

Mailing No. 77 February 12, 1979

HIRSCHFELD, HARRIS ELECTED

William C. Harris, Program Director for Structural Chemistry, NSF, and Tomas Hirschfeld, Chief Scientist, Block Engineering, have been elected to the Board of Management. They replace Prof. Jack Koenig and Dr. Ira Levin. The Society owes a vote of thanks to the retiring board members for their contributions to the Society.

COBLENTZ SOCIETY AWARDS SYMPOSIUM AND GENERAL MEETING

The Coblentz Society Awards symposium and General Meeting will take place during the Pittsburgh Conference on Thursday afternoon, March 8, 1979. Dr. Lionel A. Carreira of the Department of Chemistry, University of Georgia, recipient of the Coblentz Award, will deliver an address entitled "Development and Application of a Computer Controlled CARS Spectrometer". The Williams-Wright Industrial Spectroscopist Award will be presented to Dr. Norman B. Colthup of the American Cyanamid Company. Dr. Colthup's award address is entitled "Molecular Orbitals and Group Frequencies".

The General Meeting, which immediately follows the Awards Symposium, will consist of a brief review and discussion of the Society's activities during the past year. As a highlight of the General Meeting, Bill Fately of the Chemistry Department at Kansas State University and Ron Kagel of the Dow Chemical Company will discuss trends in vibrational spectroscopy from academic and industrial perspectives, respectively. We are anticipating an enlightening and lively afternoon.

Ira W. Levin

IN THE CADS COLUMN

Plans are underway for the best spectroscopists in the world to assemble at the annual Pittsburgh Conference. Although there are several morning and/or afternoon sessions devoted to papers on infrared spectroscopy, a highlight of the Conference for the computer assisted spectroscopy users will be the joint symposium on Fourier Transform and Computer Assisted Dispersive Spectroscopy. The symposium has been arranged through the arduous efforts of Chris Brown (CADS Group) and Jack Koenig (FT-IR Group).

The talks promise to be excellent. Looking over the schedule, we see a gamut of computer applications to infrared spectroscopy. Studies of phenomena such as chemiluminescence will be presented, a comparison of real and computer calculated spectra will be made, instrumentation used in computer assisted spectroscopy will be compared, and applications to search routines will be presented. We will hear about factor group analysis of FT-IR spectra, and we will summarize the symposium by pointing out the accomplishments and limitations of computerized infrared spectroscopy.

The various splinter groups which comprise CAS users are also holding informal meetings in conjunction with the Conference. The CADS Group is meeting on Tuesday evening from 4:30-6:00 PM in the Bob Hope Room of the Bond Court Hotel. All interested spectroscopists are invited to attend.

See you in Cleveland!

Virginia Dunning

ASTM ACTIVITIES

ASTM committee E-13 on molecular spectroscopy invites Coblentz Society members to participate in its open subcommittee meetings on March 6-7 at the Pittsburgh Conference. Details on meeting locations will be in the final program available at the conference as well as at the ASTM booth on the registration floor.

As a visitor to the meeting, you have an opportunity to comment on technical matters under consideration and to suggest projects which the committee should undertake. New task forces are formed in this way, and you may find the opportunity to accomplish public professional matters through membership in ASTM. Spectroscopic methods for use in industry, recommended techniques and calibration methods and the subjects of units and nomenclature need continuous input from those most concerned with their use.

Last year under the leadership of Kermit Whetsel, the committee completed reorganization along disciplinary lines. Clara Craver is the new Chairman and Concetta Paralusz is Secretary. Subcommittees and their Chairment are:

E-13.01	UV and Visible, Herbert Hoover, Corning Glass
E-13.02	Liaison and Communications, Jeanette Grasselli, Sohio
E-13.03	Infrared, Joseph Luongo, Bell Labs
E-13.04	Nomenclature, Clark Dehne, Capital University
E-13.05	Publications, Eugene Rosenbaum, Drexel University
E-13.06	Molecular Luminescence, Dave Teller, University of Louisville
E-13.07	NMR, Rolf Johannesen, NBS
E-13.08	Raman, Alvin Melveger, Ethicon, Inc.

Many other well-known spectroscopists also work on the committee and your participation is invited.

A major activity during 1978 was the preparation of the revision of the famous "blue book", "Manual on Practices in Molecular Spectroscopy" which will be available in late Spring from ASTM 1916 Race Street, Philadelphia, Pennsylvania. Especially timely is its basic information on quantitative procedures and microsampling as well as the extensive description of recommended practices in internal reflection spectroscopy.

Activity in 1979 is expected to emphasize coordination of the consensus standards developed in other committees such as the paint, air, water and forensic science groups. Jenny Grasselli, as chairman of E-13.02, is spear-heading this increased activity to assure reliable methodology in all ASTM procedures.

MEMBERSHIP DUES

If your membership expired in 1978, a dues card should be enclosed (your membership expiration date is printed on your address label- e.g., CR 79 means you are paid through 1979). Your prompt payment of dues (or written resignation if you don't wish to continue) will be much appreciated by those who take care of such things.

THE IDENTIFICATION OF POLYMER ADDITIVES BY INFRARED SPECTROSCOPY

SCIENCE MEDIA, a division of J. Huley Associates, Inc., announces the second program in a series, developed in a cooperative effort with the Coblentz Society and devoted to the interpretation of infrared spectra of specific classes of compounds. Richard Nyquist, of the Dow Chemical Company, has authored this unique audio guide intended for the continuing education and professional development of both student and practicing chemists.

Program materials, designed for self-study, consist of an audio cassette, approximately 60 minutes in length, a companion workbook, problem spectra, answer sheet, and text.

Following a discussion of sampling problems likely to be encountered and techniques used to isolate polymer additives for infrared analysis, the text systematically and logically assigns band positions for functional group absorptions characteristic of this class of compounds. The discussion is supplemented with a series of questions and "unknowns" for interpretation, thus emphasizing the practical aspects of spectral identification. Price $45.00.

The initial program in the series, The Interpretation of Infrared Spectra of Organosilicon Compounds, by D. A. Lee Smith, Dow Corning Corporation, has been revised to be consistent with the format of this latest program and is also priced at $45.00.

Orders may be placed directly with SCIENCE MEDIA, P.O. Box 910, Boca Raton, Florida 33432. Prices are FOB, Boca Raton.

THE SIXTH INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY - Dr. James R. Durig, Department of Chemistry, University of South Carolina, Columbia, SC 29208

Since I was Chairman of this Conference, I, of course, will have a certain amount of prejudice concerning the success of the meeting. In general, the plenary sessions were excellent with the lecturers providing a basic introduction and then a critique of the work in the area. It was particularly impressive to see the vast progress being made in the field of Coherent Anti-Stokes Raman Scattering. Workers in France and the U.S. seem to be making the most progress in this area although the Soviet Union has made a major thrust. Additionally, the utility of sampling of very small specimens appears to be a leading area in new developments in the Raman technique. In general, the analytical applications of the Raman effect were varied, and studies on thin films, flames, and microanalysis along with the Raman microprobe seemed to be areas where outstanding results have been obtained in the past two years. The meeting was strongly slanted toward those with chemical interests. This was done on purpose since the physicists in general have had their own light scattering conferences and much of the work in their area does not appeal to the chemists. Also, the Conference is sufficiently large that it cannot accommodate many more participants.

The contributed papers in my opinion were of higher calibre than those presented at the past two Raman Conferences. There were 265 contributed papers and all but 10 of these were presented by one of the authors involved in the work. There was excellent representation from the Eastern Block countries which is unusual since these scientists frequently are not able to attend international meetings. The largest session of contributed papers, of course, was on Chemical Applications. This was followed closely by the number of papers given on Ionic Crystals. Additionally, sessions were held on Molecular Crystals, Nonlinear Effects, Intensities, Polymers, Liquids and Solutions, Relaxation, and Resonance Raman Scattering. There were also sessions on Biochemistry and New Techniques along with Gases and Flames. The application of laser Raman spectroscopy to medical diagnosis was particularly interesting.

Of the 340 scientists attending this meeting, the representation from the United States was 68 scientists which was matched by a similar number from France. The United Kingdom was a close third with the rest of the participants coming more or less uniformly from other countries in Europe, Asia, Canada, and Brazil. Additionally, there were 100 Indian observers. It is my opinion that the Indian scientists benefited tremendously from this exposure to the foreign scientists. In general, the plenary lectures were well attended and the afternoon contributed papers had more or less uniform attendance.

The local organizing committee handled arrangements in a most satisfactory manner. Buses were at the airport to pick up the participants and hotel room assignments were made prior to their arrival. The projectionists were quite competent and spare bulbs and so forth were available. Most of the plenary lectures were taped. I have personally attended all of the previous International Raman Meetings and it is my opinion that the plenary lectures were the best that I have heard at any of the Conferences. Additionally, the contributed papers seemed to be of a higher quality and the exchange of ideas amongst the various participants seemed extraordinarily high. Overall, I would have to rate the scientific program as being a tremendous success and I believe it will be difficult for future international conferences on Raman spectroscopy to meet the standard that was set in the Commemoration of the 50th Anniversary of the Discovery by C. V. Raman of Effect which bears his name!

FOURIER TRANSFORM SPECTROSCOPY COURSE: IR AND NMR

Jenny Grasselli, Chairman of the Education Committee, reports that there were 22 participants in this short course given at Boston just prior to the FACSS meeting. She further reports that the course has been most effectively updated by instructing Peter Griffiths and Jim Cooper, and is now available for rent or sale on videotape cassettes. For further information, write J. G. Grasselli, SOHIO Research, 4400 Warrensville Center Road, Cleveland, Ohio 44128 or call her at (216) 575-6331.

The Coblentz Society

Statement of Income and Equity

Dec. 31, 1978

Income			
Dues		$ 1,179.96	
Spectra sales			
Sadtler		9,312.00	
Chemir - special collections		17,046.40	
Pittsburgh Conference support		1,000.00	
NSRDS, government support		2,000.00	
Interest		1,256.31	
Misc.		266.53	
			$32,061.20
Expenses			
Operating expenses: officer and committee budgets, newsletters, conferences, travel, speakers		4,435.96	
Joint Committee payback		1,652.51	
Spectral Publication Program			
Project management	1,928.00		
Special collections pub.	8,060.85		
Vol 11 development	6,912.00		
Gas phase	818.00		
Regulated chemicals	480.00		
Binders	991.25		
Misc. artwork	141.24	19,331.34	
			$25,419.81
Net Income			6,641.39
Prior Equity (Dec. 1977)			26,375.0
New Equity (Dec. 1978)			$33,016.40
Cash in Banks			
Savings		30,953.41	
Checking		2,062.99	
H. J. Sloane, Treasurer			$33,016.40