SPECTROSCOPIC FORECASTS: VARIATIONAL SPECTROSCOPY

T. Hirschfeld

We've grown accustomed to looking at IR spectra as two-dimensional pictures that display intensity as a function of wave number (or wavelength, for old-timers). Modern spectroscopic methods, with their huge SNR capabilities and their fast scan methods, may soon alter this.

When an instrument can measure 10 to 100 times as many data points in a given time, the temptation to do just this becomes irresistible as soon as some use for that additional data can be found. This is precisely what has happened in GC-IR, in which at the end of 1 hour's running time we wind up with a collection of several hundred spectra (after using computer methods for reducing the data volume). LC-IR, when invented, will no doubt do likewise.

This capability, in turn, has suggested new developments such as pyrolysis FT-IR, in which instead of GC effluent, the output of a temperature-programmed, gas-flushed oven containing the sample is measured. The use of a temperature-programmed catalytic reactor in a similar mode soon followed. Other research, in which a sample is repeatedly measured while its temperature change drives physicochemical transformations or while isotopic exchange is taking place, is the latest application of this methodology.

Such on-line spectroscopy, in which continuous scanning monitors spectral changes due to sample modifications, will see considerable growth in the future. Chemical or phase equilibria shifts, continuous titration (using a recirculator and a flow cell), photochemical or electrochemical reactions, and biochemical processes, could all be followed in this way, with time resolutions better than 1 second and favorable photometric stability. I propose the term "variational spectroscopy" as a collective noun for such techniques.

Variational spectroscopy, a child of modern spectroscopic instruments with their near instantaneous scan and integral computer, will in turn father new concepts in data handling and display. Classical methods; such as plotting a lot of spectra, will, if applied to variational spectroscopy, satisfy only chart paper and file cabinet manufacturers.

New display methods, such as advanced isometric displays (scaled, hidden line suppressed, and rotatable), contour plotting, section plotting, color gradation, or displays of third derivative or gradient will have to be
adapted from current computer technology to serve variational spectroscopy.

Variational spectroscopy, the latest outgrowth of modern infrared spectroscopy, thus illustrates a new corollary of Parkinson's law: "Curiosity expands to meet the instruments available."

FROM THE COBLENTZ BOARD MEETING

Here are a few highlights from the Coblentz Society Board Meeting that took place at the Pittsburgh Conference.

Bruce Chase was appointed the society's representative to SAS. Bryce Crawford was appointed chairman of the Lippincott Award committee.

Cooperative agreements with Chemical Transformation Systems (use of Coblentz IR Spectra), Savant (production of IR training courses), and Sadtler (Spectral Publications) were discussed. The last of these is now finalized, with the others still incomplete.

We formally elected our slate of officers: Bill Harris (President), Bob Hannah (Secretary), and Howard Sloane (Treasurer).

A financial report says we're hip deep in money (and we'll be looking for additional ways to spend it on helping the vibrational spectroscopy community).

The spectral data effort continues to go ahead nicely.

The spectral evaluation committee would like more active public participation in standard setting and in responding to suggested standards. You guys out there, please make your suggestions and responses to Peter Griffiths at Ohio University, Athens, OH.

ELECTION RESULTS

Our members have elected Al Harvey and Bob Obremski to the Board of Directors, to which their initiative and enthusiasm will be a welcome addition. It has been pointed out that keeping to our statutory deadlines in these electives would be beneficial, for which a more prompt response of the membership to the ballot mailings is desired.

Congratulations and lots of luck to Al and Bob.

INFRARED SPECTRA IN SPECIAL COLLECTIONS

The Coblentz Society now offers a set of special collections of desk books on selected areas of infrared spectroscopy. Each of these collections consists of chemically and spectroscopically evaluated spectra, printed in an easy-to-read, two-to-a-page format, and thoroughly indexed.

The available collections are:

Infrared Spectra. This is a general collection ranging over the span of chemical classes with selected examples and a considerable amount of explanatory text including general spectroscopic information.

Halogenated Hydrocarbons. These are selected for importance, and comprise a number of dilute solution spectra (for semiquantitative use) and some gas phase spectra.

Plasticizers and Other Additives. These include inorganic additives, fire retardants, and a large number of plasticizers selected for their industrial significance.

Gases and Vapors. These contain both important polluters and compounds relevant to GC-IR research and methods development.

Sales of these collections have been brisk, with most of them in their 2nd edition. Further special collections are in preparation, notably one on regulated chemicals due next year. Join in a good thing.

The hours may be long, but work can be fun.
FROM YOUR EDITOR

After producing three of these newsletters, I've arrived at the following tentative conclusions: (1) Lee Smith (our previous editor) is a 10-foot tall native of Krypton. (2) The board took advantage of my innocence when they appointed me to the job. (3) Nobody remembers deadlines. The first of each even month. Please. Pretty please? (4) I'd like the Society to give me a budget for a thumbscrew (or maybe red hot pincers) to extract contributions from prospective authors. Maybe if I take enough candid shots at meetings, I can offer nonpublication of same in exchange for contributions. (5) Bimonthly APPLIED SPECTROSCOPY issues appear near the end of their stated interval, and it then takes about a month for reprints to be mailed out to members who are not also in SAS. Since we've gone from four to six issues a year, we still break even (just). (6) When I look up and catch my breath, it's fun.

Another glimpse of Dr. Pimentel delivering his award address.

WHAT IS THE COBLENTZ SOCIETY?

The Coblentz Society is an association of persons interested in fostering the understanding and application of vibrational spectroscopy and related fields. The Society was founded in 1954 to promote communication among spectroscopists and to provide a means for improving the practice of vibrational spectroscopy, including both infrared and Raman.

It is an Affiliate Society of the Society for Applied Spectroscopy and has worked closely with many other organizations, especially those involved with standard spectroscopic reference data.

Who is Eligible for Membership?

Membership is open to persons, including students, who are interested in vibrational spectroscopy and related fields. The present membership is drawn from academic, industrial, government, and private consulting laboratories. It includes scientists interested in both dispersive and Fourier transform FT-IR techniques and instruments.

Why Should You Join?

Your participation is needed to help the Society fulfill its goals. As a member, you will have a voice in deciding what projects the Society undertakes, and you will contribute to the advancement of the field of vibrational spectroscopy.

How Do I Become a Member?

Fill in the attached application form and send with $3 for a one-year membership or $6 for a three-year membership. (Annual dues are $2, or $5 for three years; the additional $1 service fee for new members pays for the address plate.)

To become a member of the Coblentz Society, complete this form and mail along with the required amount in cash or check (payable to the Coblentz Society, Inc.).

COBLENTZ SOCIETY MEMBERSHIP APPLICATION

NAME:

AFFILIATION:

ADDRESS:

MAILING ADDRESS (if different)

One-year membership ($3)  Renewal ($2)
Three-year membership ($6)  Renewal ($5)

SEND TO:

Dr. R. W. Hannah, Secretary
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