Meetings

Spectroscopy

Advances in spectroscopy and topics as diverse as infrared-Raman, x-ray, emission, flame, ultraviolet, and nuclear magnetic resonance spectroscopy were discussed at the 14th Annual Mid-America Spectroscopy Symposium which was held in Chicago, Illinois (20–23 May).

The x-ray program featured a review of the latest application of the electron microprobe to industrial problems. Its use in the microanalysis of mineralogical investigations was discussed by Isidore Adler (U.S. Geological Survey) with particular emphasis on investigations of problems of zoning, exsolution precipitates, elemental diffusion, and the composition of coexisting phases. The complexity of the mineral makes it difficult to apply theoretical correction methods and the most precise analytical results are obtained only by the use of appropriate standards close in composition to the phases being analyzed.

B. R. Banerjee (Crucible Steel Company of America) and W. W. Welbon (General Electric Co.) pointed out that many industrial problems require a rapid semiquantitative approach plus electron and x-ray scanning photographs which are most helpful in studying compositional insight to light metallography. The versatility of the modern scanning electron microprobe has been demonstrated by (i) its use in quality control of incoming materials with a relative standard deviation of 0.6 percent, (ii) the use of electron back scatter for the identification of low atomic-weight particles, (iii) the use of the scanning microprobe for the solution and control of production processes, and (iv) the use of the unique ability of the electron microprobe to identify 10^{-12} gram of material.

Several papers brought out the expanded use of x-ray fluorescence equipment in process stream analysis and control. More widespread use of this technique has been hampered by problems of sample handling and presentation of the sample to the instrument. Recent advances in sample-handling devices for liquids, slurries, and solids were described by R. H. Munch (Monsanto Chemical Co.) and H. Calkins (Applied Research Laboratory, Inc.). An important new concept permitting the economical use of x-ray equipment for process control has also been put into operation recently. This new principle makes use of special equipment for sample-stream handling; a single x-ray instrument can be used to analyze a number of process streams on a routine basis.

A stimulating discussion arose between proponents of the Urey-Bradley force field and the generalized valence force-field methods. Both of these techniques are useful in assigning experimentally observed wave numbers and in the interpretation of the vibrational spectra of polyatomic molecules.

As stated by K. Nakamoto (Illinois Institute of Technology), one of the most fundamental problems in normal coordinate analysis is the selection of a suitable potential field to express the interatomic forces in a molecule. Although the generalized valence field is widely used by many investigators, it encounters serious difficulties in complex molecules since the number of force constants exceeds the number of observed normal vibrations. In order to circumvent the difficulty, Shimanouchi introduced the Urey-Bradley force field which consists of stretching and bending force constants, and repulsive force constants between nonbonded atoms. The number of force constants in the Urey-Bradley field is much smaller than that in the generalized valence field. In addition, the Urey-Bradley field has the advantages that (i) the force constants have a clearer physical meaning than those of the generalized valence field and (ii) they are transferable from molecule to molecule. The Urey-Bradley field, however, does not include any interaction terms between non-neighboring stretching vibrations and between bending vibrations. In some molecules, ignorance of these terms causes difficulties in adjusting force constants to fit the observed frequencies.

Discussion of the generalized valence force field using the normal coordinate treatment by the Wilson FG matrix method was presented by S. Sundaram (Illinois Institute of Technology). Work done by investigators following the method of Eliashevich and Stepanov was reviewed. The uses of the potential energy constants from the above treatments in the calculation of rotational distortion constants, coriolis constants, mean square amplitudes, bond moment derivatives, and wave numbers for isotopic molecules were discussed. Comparisons were made of the calculated values with those obtained from microwave and electron diffraction investigations. Criteria for the establishment of valid potential energy constants are: (i) that the constants yield calculated wave numbers which agree within the experimental and anharmonicity errors with each one of the observed wave number; (ii) that the constants yield calculated values of rotational distortion constants, coriolis constants, mean square amplitudes, and intensities which are within experimental error of the observed values, and (iii) that the constants agree reasonably well with the potential energy constants for other molecules with similar bond and interbond angles.

A paper entitled "A new look at light" by J. W. Robinson (Ethyl Corp.) created such a flurry of discussion and interest that it was delivered a second time the following day.

The nature of light has puzzled scientists for many years. Sometimes it behaves as if it were waves of energy and at other times behaves as if composed of many particles called photons. Scientists could never conceive that it could really be a wave and a particle at the same time. However, support for both theories has been so strong that scientists have learned to live with these two theories and, in spite of a lack of understanding of the true nature of light, have been able to make new discoveries.

Since light rays exhibit properties which are characteristic of waves and particles, this dualistic nature has been a major stumbling block in understanding the real nature of light. As a possible explanation Robinson proposed that the photon is composed of two

centers of electrical energy—one positive, one negative. These charges rotate around each other and give the photon rotational energy ($E=hv$). Movement of the whole photon gives the photon translational energy. A combination of these two energies can allow one to imagine a particle that will have properties which are wavelike but are still not waves. It is hoped that this model picture will stimulate new research into the nature of light.

M. K. Healy (Jarrell-Ash Co.) reported on the laser microprobe which has given to emission spectrochemical analysis facilities that previously have been unavailable. These include the analysis of preselected portions of any solid sample without the need to remove them from the matrix and the independence of electrical conductivity. The laser microprobe provides the excitation of a 50-micron spot in a one-shot process so that inclusions and heterogeneities may be directly analyzed.

A simple and effective attenuated total reflection unit for the ultraviolet-visible-near infrared region designed for use in a standard spectrophotometer was described by W. N. Hansen (North American Aviation Science Center). Detailed studies have been made to compare attenuated total reflection and transmission spectra. For an aqueous solution of eosin-B, which obeys Beer's law by transmission, the behavior of the visible attenuated total reflection spectrum as a function of concentration was described. Results are comparable with theoretical predictions.

The annual regional meeting was presented by the Chicago, Cleveland, Detroit, Indianapolis, Milwaukee, Niagara Frontier, and St. Louis sections of the Society for Applied Spectroscopy. In addition, a one-day meeting on gas chromatography was held by the Chicago Gas Chromatography discussion group.

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Antigens

In order to study problems on mycobacterial and fungal antigens, a conference was held at Airlie House, Warrenton, Virginia (1–3 April). Over 150 scientists from Asia, Canada, Europe, South America, and the United States attended.

Pulmonary lesions caused by *Mycobacterium tuberculosis*, unclassified mycobacteria, and fungi are indistinguishable roentgenographically. There is a great need for specific antigens for case-finding, diagnostic, and immunologic use.

Almost 40 years ago Florence B. Seibert and Esmond R. Long had identified protein as the active principle of tuberculin. Subsequently, Seibert developed purified protein derivative for use in skin testing for tuberculosis infection. For all practical purposes the standard derivative (PPD–S) has been considered specific for tuberculosis infection until the past few years. Now some of the so-called "unclassified" mycobacteria have been found to have cross-reactions to the standard derivative. The specificity has been questioned.

As papers were presented at the conference, it was evident that the relatively simple precipitation methods used to fractionate bacterial cells and culture filtrates when the derivative was first developed have been superseded to a large extent by more precise methods which have been made possible by advances in instrumentation. Electrophoresis and chromatography and new variations on these principles are being employed today as efforts continue to refine antigenic material down to the basic particle that elicits a specific immune reaction.

A combination of several methods was reported by Japanese investigators in obtaining two extracellular protein antigens of tubercle bacilli in "highly purified form." The work was done at Osaka University by Masahiko Yoneda and Yoshio Fukui. The antigens, designated as α and β, were fractionated by ammonium sulfate precipitation and purified by electrophoretic and column chromatographic techniques. Subsequent immunochemical analysis, by gel diffusion techniques, of 22 strains of mycobacteria suggested that a relationship may exist between the biological type and the distribution pattern of the two antigens in mycobacteria.

W. T. Kniker (Scripps Institute) reported using ion-exchange chromatography to separate the antigens from culture filtrates of different species of mycobacteria. After "semipure" chromatographic fractions are obtained, they can be further refined by rechromatography, and so on until the single desired antigen is obtained.

The cell wall was suggested as the proper hunting ground for antigens, in a paper presented by C. S. Cummins (London Hospital Medical College, University of London) who discussed studies showing that strains of mycobacteria, corynebacteria, and nocardia have the same sugar and amino acids in their basic cell-wall structure. Cummins has found that strains with this type of cell wall appear to contain at least one antigenic component in common. Located in the wall, the component can be detected in an agglutination by using a suspension of cell-wall fragments as antigen. Cummins suggested that bacterial anatomy would be the basis for a fruitful search for mycobacterial and related antigens.

A two-stage process was described by Richard S. Farr (Scripps Clinic and Research Foundation). Farr's process, briefly, was to label cell-free extracts with radioactive iodine and to use the labeled antigen precipitate to measure the binding capacity of serums for the bacterial extract. In a series of serums from 88 tuberculosis patients, he reported that 37 had a higher binding capacity than was found in any of 63 nontuberculosis patients.

A paper by a veterinarian called attention to the importance of antigens specific for each species of mycobacteria. W. LeRoy Mallman (Michigan State University) reported isolating unclassified mycobacteria from a herd of swine raised at the university. The possibility that these organisms cause a reaction to the tuberculin test cannot be ignored and could mean that many cattle slaughtered on the assumption that they are tuberculous are actually not capable of transmitting the disease to man.

Development of two vaccines effective against experimentally produced coccidioidomycosis in mice and monkeys was reported by John L. Converse (U.S. Army Biological Laboratories, Fort Detrick, Md.). One of the vaccines is made from dead spores of *Coccidioides immitis* and the other from live spores. The vaccine killed by formalin did not appear to give as great a protection as the live vaccine.

One paper was based on studies in leprosy. R. J. W. Rees (National Institute for Medical Research, London) reported serological studies on 75 patients with different types of leprosy. By means of agar-diffusion techniques, precipitating antibodies to a variety of mycobacterial antigens have been detected in patients' serums. The results indicate that different types of leprosy can be identified by the pattern of antibodies.