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**ABSTRACTS
OF
PAPERS**

Fifth Annual

Rocky Mountain

Spectroscopy Conference

Sponsored By

Rocky Mountain Section

Society For Applied Spectroscopy

THE OLIN HOTEL

Denver, Colorado

August 6 - 7, 1962

August 6 – Monday Morning

9:05 AM – Speaker, Mr. L. M. Cartwright

"Elemental Analysis by Neutron and Photon Activation"
by L.M. Cartwright, Peter Gray, and D. J. Veal

Abstract

The progress made to date in our laboratories on the application of activation techniques to routine elemental analysis is described. Rapid, sensitive and accurate methods for the determination of aluminum, oxygen, chlorine, nitrogen and selenium which have reached the routine or near-routine state, are briefly discussed. The time per analysis for these methods is ^{1/4} to 1/2 hour and the sensitivities achieved are all in the several hundred parts-per-million range or less. Brief descriptions are given of the methods for the determination of fluorine, silicon, iron, phosphorus, vanadium and nickel which are in an early development stage. Numerous other elements are listed whose determinations could be reduced to routine practice should the need arise.

NOTES

August 6 -- Monday Morning
9:25 AM -- Speaker, James Perry

"Electron Spin Resonance Study of Radiation Damage Magnesium Hypophosphite Hexahydrate"

by James Perry and Melvin W. Hanna

Abstract

An ESR study of irradiated $\text{MgH}_2\text{PO}_2 \cdot 6\text{H}_2\text{O}$ has shown that the long-lived free radical HPO_2 is produced. Hyperfine interactions of both the proton and phosphorus nuclei have been studied as a function of the orientation of the applied magnetic field. The results are to be contrasted with those recently obtained on irradiated Mg HPO_3 (1,2) in that the p_{31} hyperfine splittings are considerably smaller. The significance of these results in terms of orbital hybridization and spin correlation will be discussed.

(1) M.W. Hanna and L.J. Altman, *J. Chem. Phys.*, 36, 17788 (1962).

(2) A. Horsfield, J.R. Morton and D.H. Whiffen, *Mol. Phys.* 4, 475 (1961)

NOTES

August 6 – Monday Morning

9:45 AM – Speaker, A. J. Mitteldorf

"Instrumentation and Some Typical Applications in the Grazing
Incidence Ultraviolet"

by A. J. Mitteldorf

Abstract

A brief survey of the state-of-the-art in sources, gratings, detectors, filters, spectrographs and applications is given. Particular emphasis is placed on the GISMO (Grazing Incidence Spectrometer Monochromator) manufactured by Spex Industries. Its unique feature permitting direct readout in angstroms at varying angles of incidence is discussed from the standpoint of usefulness.

NOTES

August 6 – Monday Morning
10:25 AM – Speaker, Dr. Wilbur Kaye.
"Advances in Par Ultraviolet Spectroscopy"
by Wilbur Kaye

Abstract

August 6 – Monday Afternoon

11:30 PM—Speaker Peter J. Berkeley

"A Nuclear Magnetic Resonance Study of *Hydrogen* Bonds to Nitrogen"
by Peter J. Berkeley and Melvin W. Hanna

Abstract

The position of the proton resonance of chloroform has been determined as a function of concentration in acetonitrile, pyridine and N-methylpyrrolidine. On the assumption that a single equilibrium exists between monomeric species and a hydrogen-bonded dimer, an equilibrium constant for association, and a chemical shift for the pure H-bonded species, have been derived. The results will be interpreted with regard to the influence of the type of hybridization of the basic nitrogen on the H-bond strength and on the magnitude of the H-bond shift. The interrelation between anomalous solvent effects, ring current and diamagnetic anisotropy effects will be discussed.

NOTES

August 6 — Holiday Afternoon
1:50 PM — Speaker, **William L.** Baun

"The Use of Various Ion Sources in a Double Focusing Mass Spectrograph for Organic Solids Analysis"

by William L. Baun, Neil Hodgson, and Michel Desjardins

Abstract

Mass spectra of organic compounds are invaluable for use in qualitative and quantitative analysis and in structure elucidation of organic compounds. Unfortunately, many solid organic compounds do not give representative spectra using conventional ion sources. This work reports the use of various sources and techniques to gain information on stable solid organic compounds. A multi-source double focusing mass spectrograph of the Mattauch type is used in this work with a heated solids inlet, Knudsen cell, and high frequency spark available for ionization of any solid sample. The spectrograph may also be used as a spectrometer by converting from a photographic plate to an electrometer or photomultiplier detector for more accurate intensity measurement. Mass spectra of several organic solids are shown with emphasis on biological compounds. Spark spectra are shown for stable aromatic compounds and phenyl-metal compounds.

NOTES

August 6 — Monday Afternoon

2:10 PM—Speaker, Mr. Francis R. McDonald

" A Comparison of the Infrared Spectra of Benzo (b) Thiophenes and Benzenes "

by F.R. McDonald and Glenn L. Cook

Abstract

The infrared spectra of benzo (b) thiophene and 17 of its alkyl homologs have been compared with spectra of substituted benzene. If benzo (b) thiophene is considered to be a 1,2-disubstituted benzene, then the 17 alkyl homologs are divided into groups. Three are in the 1,2-disubstituted group; seven are in the 1,2,3-trisubstituted group; five are in the 1,2,4-trisubstituted group; two are in the 1,2,3,5-tetrasubstituted group. The spectra are discussed in relation to the position of the substituent on the benzene ring.

The 5- to 6-micron region, the 8- to 10-micron region and the 11- to 15-micron region of the infrared spectra are used throughout the literature to show positions of substituents on the benzene ring. These same regions of the infrared spectra of the benzo(b)thiophenes are discussed for the four groups.

Patterns in the 5- to 6-micron region, for the overtone and combination bands, match those for benzenes. Bands in the 8- to 10-micron region are assigned to the C-H in-plane deformation modes. Additional bands in the region are explained by the effects of the substituents. Bands in the 11- to 15-micron region are assigned to the C-H out-of-plane deformation modes. It can, therefore, be concluded that the thiophene ring of the benzo(b)thiophene does not change the assignment of bands used to indicate the positions of substituents on the benzene ring.

NOTES

August 6 -- Monday Afternoon

2:50 PM -- Speaker, Dr. D. S. Erley

"Infrared Analysis of Normal and Pathologic Blood Serum by
Statistical Methods"
by Dr, D. S. Erley

Abstract

The infrared examination of blood serum and other body fluids initiated in this laboratory in 1956, has led to the aquisition of a large number of spectra of both normal and pathologic blood serum. Several factors lead to variations in the spectral pattern observed. These are:

1. Small individual differences between normal subjects.
2. Larger differences in composition arising from pathologic conditions.
3. Variations in the absolute thickness of the serum layer scanned and in relative thickness of the compensating water layer.
4. Photometric errors which may be aggravated by the low infrared transmission of water solutions.

In order to evaluate the infrared analysis of blood serum as a diagnostic tool, it is necessary to separate the differences caused by "2" above, from other sources of variation. The effects of film thickness differences may be minimised by comparing absorption band ratios rather than the absorbances themselves. The other sources of "error" have been evaluated on a statistical basis.

This evaluation has been facilitated by two programs written for an Autonetics "Recomp III" computer. One program accepts absorbance data from normal blood serum spectra and computes 36 "normal serum absorption band ratios, plus the standard deviation of each ratio. The second program compares the 36 absorption band ratios of a pathologic sample with the 36 normal ratios stored in memory, and prints out those ratios which deviate significantly. A brief description of the two computer programs will be presented, as well as examples of their application to the analysis of blood serum.

NOTES

August 7 - Tuesday Morning

8:50 AM - Speaker, H. J. P. Lyon

"Analysis of Rocks and Minerals "by Reflected Infrared Radiation"
by R.J.P. Lyon and E.A. Burns"

Abstract

The earliest studies of minerals by reflected and emitted infrared radiation were those of Goblentz (1900-1910). Since then mineralogical uses of reflected infrared radiation have been restricted primarily to studies of glass, and to minerals like quartz and cristobalite which play a prominent part in the understanding of glass structures. Similarly, infrared emission studies are restricted almost exclusively to ceramics and refractories. This paper deals with the reflected infrared analysis of several common minerals and rocks. A brief review of the optical principles involved, and the typical spectra to be obtained from quartz plates, fused silica and glasses will be made and recent spectral data from mineral and rocks will be examined. Similarities and differences between absorption and reflection spectra for the same materials will be discussed, and problems encountered in the calculations of composition (modal analysis) will be indicated.

Applications to nondestructive testing of polished rock surfaces (or gems) and to the calculation of ambient-temperature emissivity curves for rocks will be shown. Such spectral emissivity curves are an important prerequisite for the remote mapping of the lunar and other planetary surfaces.

NOTES

August 7——Tuesday Morning

9: 10 AM—Speaker, David. A. Duke

"Infrared Investigation of the Olivine Group Minerals"
by David A. Puke and James D. Stephens

Abstract

Natural and synthetic minerals of the olivine group were investigated using infrared absorption techniques in the frequency range 4000 cm^{-1} to 530 cm^{-1} . The KBr pressed-pellet technique was used and the spectra were obtained on a Perkin-Elmer model 421 double beam, grating spectrophotometer.

In general, five absorption bands are noted. The frequency of each band either increases or decreases depending on the cation which bonds together the SiO_4 tetrahedra. The frequency shift is different for each of the absorption bands. The changes in frequency of the bands are related empirically to differences in the mass, ionic radii, and electronegativities of the various substituent cations.

Olivine group members studied include the following cation pairs Mg-Fe, Fe-Mn, Mg-Ca, Mg-Mn, Ca-Mn, Mg-Ni, and Mn-Ni.

The general position of the bands is calculated by assuming that they are caused by vibrations within the SiO_4 tetrahedra. The symmetry properties of the olivine unit cell reveal the distortion of the tetrahedral symmetry of the SiO_4 to a point group symmetry of Cs. Analysis of the group character tables reveals that the observed absorption bands are explained by this symmetry distortion.

NOTES

August 7 - Tuesday Morning
9:30 AM _____ Speaker A.R. Ronzio

"Chemical Composition of Old-Time Smelter slags from Sites
in Colorado"
by A.R. Ronzio and M.L. Salmon

Abstract

Analyses of old-time smelter slags by x-ray spectrography indicated residual concentrations of the metals sought in the smelting of the ores and the types of fluxes used in these early processes.

NOTES

August 7 - Tuesday Morning
9:45 AM - Speaker, M.L. Salmon

"Correlation of Chemical Composition and Color of Turquoise Specimens"
by A.R. Ronzio and M.L. Salmon

Abstract

X-ray spectrographic studies of turquoise specimens revealed trends of elemental composition that can be correlated with the color of the specimens.

The non-destructive nature of x-ray spectrography is important because the gem quality materials can be directly examined with no resultant damage and specimens can be checked prior to processing to detect the use of artificial coloring to upgrade the value of the mineral.

NOTES

August 7 – Tuesday Afternoon

1:30 PM——Speaker, Dr. John A. Norris

"Research and Development Using Photoelectric Spectrometric Equipment"

by Dr. J. A. Norris

Abstract

The use of certain electronic devices in combination with commercially available spectrometric equipment has broadened and speeded research in spectrochemical analysis. With this type of equipment it is possible to actively study phenomena such as element volatilization time and rate. The instantaneous graphical presentation of this type of information enables the investigator to carry out a more complete study of the variables encountered in procedure development. The use of spectrometric equipment also allows the acquisition of larger amounts of statistical data which permits greater refinement of experimental variables. Examples of this type of equipment and its use in spectrochemical procedure development will be given.

NOTES

August 7 — Tuesday Afternoon

1:50 PM — Speaker, Harold F. Emery

"A Direct Reading Spectrometer of Modern Design"
by Harold F. Emery

ABSTRACT

A new Direct Reading Spectrometer providing flexibility and compactness is described. A group of modules can be assembled in a variety of combinations to receive light from one analytical gap. Included are an Air Spectrometer, a Vacuum Spectrometer and a Spectrograph. A 3-meter grating with a folded Rowland Circle mount is utilized in the Air Spectrometer. Optical alignment is assured through the use of the "Optical Interlock" and a dispersion compensator. The evacuated volume of the Vacuum Spectrometer is minimized by the range doubling optical system. Spark, low voltage AC arc, and DC arc are provided in the source unit. The measuring system, which is sequential in operation, provides facilities for the use of multiple internal standard lines and dark current correction and is contained in a group of plug-in modules. Switching takes place at a low impedance levels and amplification is at 400 cycles. Performance data will be presented.

NOTES

August 7 - Tuesday Afternoon
2:10 PM——Speaker W.G. Schrenk

"Some Factors Involved in Flame Photometric Analysis for Trace Elements in Biological Materials"
by W. G. Schrenk

Abstract

The problems of the analytical flame photometry of trace elements in biological samples may be summarized in three general groups, (1) sensitivities, (2) interferences, and (3) sample preparation. For a satisfactory analytical procedure all three categories must be satisfactorily controlled.

The sensitivity of a spectral line or band excited by a flame can be controlled in several ways, including the following: (1) Proper line or band selections, (2) Flame dimensions, (3) Aspiration rate, (4) Flame temperature, (5) Spray particle size, (6) Flame area used, and (7) Chemiluminescence.

Interference effects which may influence the proper development of flame methods may include: (1) Adjacent spectral line or band interference, (2) Continuous background radiation, (3) Instrument resolving power, (4) Self-absorption, (5) Cation-cation interactions, and (6) Cation-anion interactions.

Each of the above named items in each category will be discussed and most will be illustrated with examples. Emphasis will be placed on enhancement effects due to flame temperature, as a result of using organic solvents, on limited area flame photometry and on chemiluminescence phenomena. Concentration methods will be discussed for certain elements when other enhancement procedures fail.

Interference effects which will be emphasized and illustrated with examples include spectral line and band interference, cation-cation interactions and cation-anion interactions.

Proper sample preparation of biological materials is necessary if precise analytical results are to be expected. In some cases sample preparations are very simple and in others very complex. Examples will be cited concerning problems encountered due to the presence of proteins, carbohydrates, fats, and minerals. Precise flame procedures must account for these factors or they must be removed from the test solutions aspirated into the flame.

NOTES

August 7 - Tuesday Afternoon

2:30 PM——Speaker, Mr. Carl J. Leistner

"The Determination of Trace Elements Using the Vacuum Cup
Solution Technique"
by Carl J. Leistner

Abstract

The paper will describe the use of the Zink Vacuum Cup Electrode for the spectro chemical analysis of trace amounts of metallics in aqueous solutions, utilizing an OH band component in the O-O band system heading at 3064 A as an internal standard line.

NOTES

August 7 – Tuesday Afternoon
2:50 PM – Speaker, A. J. Mitteldorf

MOVIE

"The Use of Atmospheres In Emission Spectroscopy"

Abstract

This film describes three relatively new techniques of excitation in emission spectroscopy utilizing gases other than air.

A very striking series of scenes is depicted illustrating the stabilizing effects of the Stallwood Jet. Another section of the film shows the use of the newer Plasma Jet, and a third section describes the controlled atmosphere chamber which, in essence, is based on the work of Dr. Fassel at Iowa State University.

NOTES