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Article 1

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17th Annual Rocky Mountain Spectroscopy Conference

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17th Annual Rocky Mountain Spectroscopy Conference

Abstract

Final program and abstracts from the 17th annual meeting of the Rocky Mountain Spectroscopy Conference, sponsored by the Rocky Mountain Section of the Society for Applied Spectroscopy. Held in Denver, Colorado, August 4-8, 1975.

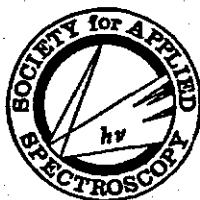
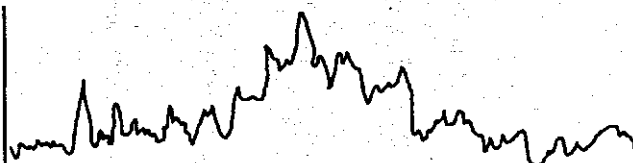
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**17TH ANNUAL
ROCKY MOUNTAIN
SPECTROSCOPY
CONFERENCE**

FINAL PROGRAM – ABSTRACTS

AUGUST 4–5, 1975

**BROWN PALACE HOTEL
DENVER, COLORADO**

Sponsored by the
ROCKY MOUNTAIN SECTION
of the
SOCIETY FOR APPLIED SPECTROSCOPY

Welcome to Denver

Officers of the Rocky Mountain Section Society for Applied Spectroscopy

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Ball Brothers Research Corporation
Boulder, Colorado

Chairman-Elect: Robert Heidel
U.S. Geological Survey
Denver, Colorado

Secretary: Jean R. Gaines
Rockwell International
Golden, Colorado

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Ingrid Matzner
Denver, Colorado

General Information

Sponsor

This year's Annual Rocky Mountain Spectroscopy Conference continues the well established tradition of friendly exchange in an informal atmosphere. The papers of the program cover a broad sampling of the field of spectroscopy, some of the latest instrumentation and equipment will be on exhibit, and the banquet promises to be a relaxing diversion.

The Rocky Mountain Section of the Society for Applied Spectroscopy welcomes all of you to Denver and requests your full participation in the conference.

Registration

Registration badges will be necessary for admission to all sessions. Registration fees are as follows:

All conferees (except students)	\$15.00
Students (full time)	\$ 4.00
Banquet	\$ 6.00

Conference Mixer and Banquet

The conference banquet will be held Monday evening, August 4th at 7:00 p.m. in Ballroom B. Preceding the banquet there will be a hosted cocktail hour (admission by banquet ticket) from 6:00 to 7:00 p.m. Tickets for the banquet will be available at the registration desk until noon, Monday.

Banquet Menu

Fruit Supreme
Mixed Green Salad with Club Dressing
Roast Baron of Beef
Baked Potato
Buttered Asparagus Spears
Frozen Mocha Ice Cream Pie
Coffee—Tea—Milk

In recognition of service to the RMS-SAS, the 1975 Outstanding Service Award will be presented to Mr. Bill J. Wiginton of Marathon Oil Co. Mr. Wiginton is past chairman of both the Rocky Mountain Spectroscopy Conference and RMS-SAS.

After the presentation, Mr. Joe K. Lange of Chevron Research, Denver, will present a dual slide projector show entitled "Symphony in Nature" accompanied by pre-recorded music. Most of the slides were taken in the national parks of the western United States. The slides and music are coordinated in a fashion to produce beautiful montages and, at times, dramatic effects.

Mr. Lange is a graduate of Colorado School of Mines with a degree in geophysics. He is first Vice President of the Englewood Camera Club, President Elect of the Colorado Council of Camera Clubs, a member of the Photographic Society of America (PSA). He is a four-star color slide exhibitor in the nature slide division of PSA and a three-star exhibitor in the nature print division.

Exhibits

Current state-of-the-art instruments and equipment will be on display outside the auditorium. Exhibitors include:

- American Instrument Company
- Beckman Instruments
- The Buhrke Company
- Diano
- KEVEX Corporation
- Siemens Corporation
- Tracor Northern Incorporated
- U.S. Geological Survey

Coffee Breaks

Coffee and rolls will be served at the morning recesses and coffee and coke at the afternoon recesses in the exhibit area. This is supported in part by the following companies:

- ORTEC Incorporated
- Perkin-Elmer Corporation
- Technical Equipment Corporation
- Van Waters & Rogers Scientific

DRI X-Ray Conference

The 24th Annual Denver Conference on Applications of X-Ray Analysis will be conducted at the hotel August 6, 7, & 8. For additional information contact C. O. Ruud, Metallurgy and Materials

Science Division, Denver Research Institute, University of Denver, Denver, Colorado 80210. Phone (303) 753-2141.

Inquiries

For additional information on the RMS-SAS Conference, address inquiries to: Stephen E. Valente, Custom Chemical Co., P.O. Box 5303 T.A., Denver, Colorado 80217. Phone (303) 477-1676.

Conference Schedule

All sessions will be held in Ballroom A.

Monday Morning (I)

Bill McCarty, Session Chairman, Marathon Oil Co., Littleton, Colorado.

8:30 Welcoming Remarks

Robert Heidel, RMS-SAS Chairman-Elect.

8:35 Infrared-to-Visible Conversion in Er^{+3} Doped Crystals

D. G. Ettinger and T. M. Niemczyk, Department of Chemistry University of New Mexico, Albuquerque, New Mexico 87131.

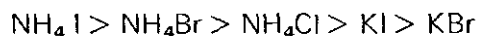
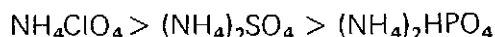
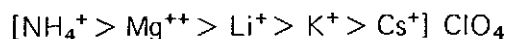
Rare earth doped fluorides, capable of acting as upconverters, have been prepared and studied in our laboratory. These crystals, when excited with infrared radiation (~ 970 nm) show visible luminescence bands around 500 nm and 660 nm. Fluoride type phosphors are prepared by precipitating the mixed fluorides from an acidic solution containing the appropriate ratio of dopant to host lattice ions. The mixture is washed and then fused at high temperature (~ 1200 °C) in a vacuum furnace designed and constructed in this laboratory. The resulting compounds are ground to a fine powder and, using glycerine as a bonding agent, a small amount of this powder can be positioned in the measurement apparatus. Pulsed or continuous IR excitation is provided by a gallium arsenide diode (Texas Instrument TIXL16) or a tungsten halide lamp source.

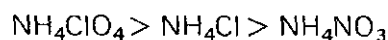
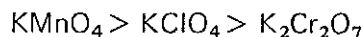
Data will be presented to justify a proposed mechanism for the overall luminescence process. In addition, data representing the temperature dependence, the kinetic behavior and matrix effects will be discussed.

8:55 DSC and TG Study of the Effect of Inorganic Additives on the Thermal Stability of Delrin and Celcon

A. S. Tompa and D. M. French, Propellant Sciences Department, Naval Surface Weapons Center, White Oak Laboratory, Silver Spring, Maryland 20910.

The effect of additives on the thermal decomposition of Delrin and Celcon polyacetals was investigated. The order of decreasing thermal stability of the polyacetal may be correlated with increasing acid strength of the additive anion or decreasing basic strength of the base of the additive cation. It was found that keeping the anion constant, the order of instability with cations increases going up a group and across a period in the Periodic Table; keeping the cation constant, the order with anions increases going down a group and across a period; with oxidizing agents, keeping the cation constant the order increases with the oxidation potential. Oxyanions are more effective in decreasing stability because the presence of additional oxygen atoms increased the ionic potential of the element in the anion and therefore the acid strength of the anion. Peroxyanions are still more effective in decreasing stability because when heated they liberate free radicals and oxygen. Methyl substituted cations are less effective in decreasing stability because methyl groups are base strengthening. These conclusions are based on the following observations on the effect of additives on decreasing the thermal stability of polyacetals:





The studies indicate that thermo-gravimetric analysis (TG) offers a novel method for distinguishing the relative acid strength of many inorganic compounds by the single measurement of the relative effect the compound has on lowering the thermal stability of Delrin in an inert atmosphere. Activation energies were calculated for some of the decomposition reactions.

9:15 Use of Multiple Regression Analysis in UV-Visible Spectrophotometry

William E. McDermott, Department of Chemistry
USAF Academy, Colorado 80840.

Conventional procedures for the resolution of interfering species in UV-visible spectrophotometry involve the determination of separate calibration curves for each species at two wavelengths. Measurement of the unknown absorbance at these wavelengths allows the mixture to be resolved via the solution of two simultaneous linear equations. This paper discusses the application of spectrum stripping techniques to the resolution of interfering species in UV-visible spectrophotometry. In this method the absorbance is measured for each species as a function of wavelength and a multiple regression analysis used to determine the concentrations in the mixture. The accuracy and sensitivity is compared with the conventional method and the extension to N-component mixtures discussed. This technique is especially suitable for use with spectrophotometers having direct digital readout. Analysis may be performed via a calculator or computer.

9:35 Spectroscopic Studies of IrF_6

Elliot R. Bernstein and *John D. Webb*, Chemistry Department, Colorado State University, Fort Collins, Colorado 80521.

Hexafluorides are interesting for two reasons: they have many degenerate electronic states which should allow study of the Jahn-Teller effect, and they form molecular crystals, allowing extension of theories formulated for organic molecular crystals.

Previous workers^{1, 2} have taken spectra of neat crystals of IrF_6 ; their spectral assignments indicate a strong dynamic Jahn-Teller effect in several of the excited states. The present experiments are low temperature (1.8K) absorption spectra in the visible and near IR of neat and mixed crystals of IrF_6 . The hosts are either UF_6 , WF_6 , or MoF_6 . The results will be discussed with emphasis on new assignments which are indicated by the mixed crystal data. The new assignments show that the Jahn-Teller effect is much smaller than previously believed.

¹ Brand, Goodman, Can. J. Phys. 46, 1721, 1968.

² Brand, Goodman, Weinstock, J. Mol. Spec. 37, 464, 1971.

9:55 Coffee Break

Monday Morning (II)

Keith Grossaint, Session Chairman, Rockwell International, Golden, Colorado.

10:15 The Effect of pH on the NMR Spectrum of Tetracycline

G. L. Asleson and C. W. Frank, Dept. of Chemistry, University of Iowa, Iowa City, Iowa 52242.

The carbon signals for tetracycline hydrochloride in a 50/50 DMSO:water system have been shown to be dependent on the pH of the solution. Shifts of up to 16 ppm were observed for 18 of the 21 tetracycline signals. Graphs of chemical shift vs pH are similar to titration curves with a distinct break for the first pK_a and an overlap of the second and third pK_a s (4.4, 8.1, and 9.8). These curves can be used to corroborate the ^{13}C NMR signal assignment and to calculate the dissociation constants.

10:35 Nuclear Spin-Lattice Relaxation Times in Tar Sands

F. P. Miknis, A. B. Denison¹, and S. M. Dorrence, Energy Research and Development Administration, Laramie Energy Research Center, Laramie, Wyoming 82071.

Nuclear spin-lattice relaxation times, T_1 , of a tar sand core, and a bitumen extracted from the core, have been measured in the temperature range 250 °K to 500 °K at resonant frequencies 20 and 60 MHz. At low temperatures, the relaxation times of the core, and bitumen showed similar temperature dependencies with a pronounced minima occurring at about 330 °K in both samples. For temperatures greater than 330 °K, the bitumen exhibited non-exponential relaxation. Possible relaxation mechanisms for the observed temperature dependence on the tar sands T_1 's will be discussed.

¹Permanent address University of Wyoming, Physics Department, Laramie, Wyoming.

10:55 Characterization of Oil Combustion Products from Utah Tar Sands Using Mass and Infrared Spectroscopy

F. D. Guffey and S. M. Dorrence, Energy Research and Development Administration, Laramie Energy Research Center, Laramie, Wyoming 82071.

The demand for additional energy has brought attention to alternate sources of fossil fuels such as tar sands. To use these resources to their fullest potential it is necessary to characterize the products obtained by different recovery methods. Narrow boiling distillate cuts were prepared from the combustion products of P. R. Spring and Asphalt Ridge, Utah tar sands for characterization by mass and infrared spectroscopy.

Use of these two forms of spectroscopy provided characterization of the distillate cuts. Functional group types and molecular weight ranges were obtained. Results obtained on the distillate cuts of product oils from reverse combustion of both tar sands were compared with corresponding results obtained following forward combustion. These results were contrasted with the results obtained

on the total product oil to demonstrate the need for narrow boiling distillate cuts to provide a significant characterization of the products.

11:15 Role of Excited States of Ions in Fragmentation Processes in a Mass Spectrometer

J. H. Weber, R. E. Ellefson¹, and A. B. Denison², Energy Research and Development Administration, Laramie Energy Research Center, Laramie, Wyoming 82071.

Fragmentation processes in mass spectrometry have been the subject of numerous investigations in recent years. Various techniques, such as; metastable transitions, isotopic labelling, ion energetics, and ion kinetic energy mass spectrometry, have been used to probe the fragmentation processes. We present here a method for studying excited state processes via a double electron impact-optical radiation spectroscopy. Experimental results are presented for n-pentane and several other small molecules.

¹Permanent address Mound Laboratories, Miamisburg, Ohio.

²Permanent address University of Wyoming, Physics Department, Laramie, Wyoming.

11:35 Lunch

Monday Afternoon (III)

Frank Schweitzer, Session Chairman, Coors Spectrochemical Laboratory, Golden, Colorado.

1:15 A Method for the Statistical Determination of Impurity Concentrations in Standard Materials for the Evaluation of Analytical Standards

Calvin J. Martell, William M. Myers, Gary L. Tietjen, and Myrle M. Horita, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544.

A statistical method has been applied to analytical data collected from a plutonium exchange program. The objective is to accurately determine metal impurity concentrations in plutonium metals using data from four different methods of analysis. These well characterized standard materials are then used to evaluate four types of analytical standards for the carrier-distillation analysis of

PuO₂. The items evaluated include: (1) the effect of dilution on an impure plutonium sample; (2) the effect of the use of an internal standard; (3) the degree fit to apply to standard data; and (4) which one set of standards most accurately determines the impurities studied. The statistical method described can be applied to any standard material where sufficient data are available.

1:35 Determination of Atmospheric Trace Contaminants

D. L. Dick and R. K. Skogerboe, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523.

Methods for the collection and determination of several atmospheric trace contaminants have been characterized. The applicability of these to the determination of trace and ultratrace contaminants will be critically discussed.

1:55 Characterization of Interference Effects in Non-Flame Atomic Absorption

G. W. Johnson and R. K. Skogerboe, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523.

It has been determined that the magnitude of an atomic absorption signal is often repressed by the presence of common anions in the analytical solution. These interferences have been characterized for several metal-anion combinations and means have been developed for eliminating them. The nature of the effects and the corrective procedures required will be discussed.

2:15 Optimizing Atomic Absorption Analysis for the Determination of Rhenium and Hafnium in Tantalum Alloys

Joseph S. Rudolph, Westinghouse Electric Corp., Research Laboratories, 1310 Beulah Road, Pittsburgh, Pennsylvania 15235.

Increasing application of atomic absorption has been made to the determination of refractory elements principally because high sensitivity has been obtained with the premixed nitrous oxide-acetylene burner. When maximum sensitivity is

required, optimization of the atomic absorption variables; e.g., fuel to oxidant ratio, burner position, solvent and instrument conditions is critical. An investigation to determine the effect of sample composition, the addition of ethanol to the solvent, fluoride ions and sulfate ions showed each to have a dramatic effect on the absorbance and detectability of rhenium and hafnium. Analytical data will be presented for the determination of 1% rhenium and 1% hafnium in tantalum alloys containing 8% or 12% tungsten. Comparative X-ray spectrochemical data shows that accurate atomic absorption determinations of rhenium and hafnium can be made in these alloys.

2:35 Coffee Break

Monday Afternoon (IV)

Jim H. Weber, Session Chairman, Energy Research and Development Administration, Laramie Energy Research Center, Laramie, Wyoming.

2:55 Analysis of Copper, Iron, and Cadmium in Plant Material by Atomic Absorption Spectroscopy

Duane R. Boline and W. G. Schrenk, Department of Chemistry, Kansas State University.

A method of analysis for copper, iron, and cadmium in plant material by atomic absorption spectroscopy has been investigated. The digested samples are diluted with an alcohol-water mixture and aspirated directly into an air-acetylene flame. Interference due to the presence of calcium, sodium, potassium, phosphate, sulfate, perchlorate, and the other two elements included in the study was found to be negligible in the analysis for each metal. A sensitivity of 0.05, 0.08, and 0.05 mg/l; and a detection limit of 0.008, 0.01, and 0.01 mg/l have been found for copper, iron, and cadmium respectively. The analysis results obtained by this method have been compared to the results obtained by the analysis of identical samples by the A.O.A.C. colorimetric methods.

3:15 Indirect Determination of Sulfate in Water by Atomic Absorption

O. Karmie Galle and Lawrence R. Hathaway, Kansas Geological Survey, 1930 Avenue "A" Campus West, University of Kansas, Lawrence, Kansas 66044.

There are numerous references which describe the determination of sulfate or sulfur in a variety of materials by atomic absorption. However, there are no references in the English literature which describe such a method specifically for water. The method outlined in this paper was adapted from one developed for the determination of sulfate in textiles. Barium sulfate is precipitated and the excess barium determined by A.A. The purpose of this report is to present some typical results which can be obtained using atomic absorption methods as compared with gravimetric methods. Standard deviations and relative standard deviations from a series of analyses will be presented.

3:35 Determination of Ultratrace Amounts of Silver in Precipitation

J. N. Viets, J. D. Sheaffer, and R. K. Skogerboe, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523.

A simple, direct, and sensitive method for the determination of silver in precipitation by non-flame atomic absorption will be described. The advantages of the method over others in use will be discussed.

Tuesday Morning (V)

A. Tennyson Myers, Session Chairman, U.S. Geological Survey, Denver, Colorado.

8:30 Inductively-Coupled Plasma--Optical Emission Spectrometry: Application to the Determination of the Major and Minor Elemental Composition of Minerals

E. L. DeKalb, E. M. Layton, Jr., and V. A. Fassel, Ames Laboratory USAEC and Dept. of Chemistry, Iowa State University, Ames, Iowa 50010.

An induction coupled plasma has been used as the excitation source for the quantitative

determinations of the major and minor elemental compositions of mineral samples. A multichannel direct-reading spectrometer was used to detect and quantify the characteristic radiation of the several elements measured. Putverized samples were rendered soluble by use of a lithium metaborate fusion followed by dissolution in dilute nitric acid.

A significant advantage of this analytical approach is the nearly complete absence of inter-element effects. Congruent linear analytical calibration curves were obtained from a wide variety of standard samples, including USGS silicate rock standards, and US Bureau of Standards cements, limestones, iron ores, glasses, and phosphate rock. The results thus far obtained clearly indicate that rock and mineral specimens of nearly any type can be accurately analyzed with only one set of analytical curves. Reasons for this lack of inter-element effects will be discussed.

8:50 Optical Emission Spectrochemical Analyses with the Hollow Cathode

J. D. Johnson, Spectrogram Corporation, 385 State Street, North Haven, Connecticut 06473.

The operation and control of a demountable hollow cathode source for routine optical emission analyses is described. The high resolution and negligible self absorption of the source yields a wider dynamic range than most emission sources. Since the components of a sample, deposited on the inner wall of the cathode, undergo many cycles of sampling, excitation and redeposition, the source is ideal for the multielement analysis of samples of one milligram or less.

A number of sample preparations are shown, including filtration, evaporation and in situ ashing in cathodes. The analysis of samples essential to life is demonstrated; namely—oil, water and blood.

9:10 Rapid-Scanning Spectroscopy of Metal Combustion

J. C. Moulder, D. S. Lund, and A. F. Clark, Cryogenics Division, Institute for Basic Standards, National Bureau of Standards, Boulder, Colorado 80302.

The time-resolved emission spectra of metal specimens burning in oxygen are obtained using a rapid-scanning spectrometer and digital storage techniques. After ignition by a CO₂ laser, reactant and product species can be identified and their development monitored by their line and band emissions between 300 and 1100 nm, with a time resolution of 10 ms. Alloy constituents or impurity lines are also observed, sometimes in absorption. Spectra will be given for several different metals and alloys and line ratios will be compared to known thermal excitation spectra. Scans over as much as 400 nm were obtained permitting observation of an anomalous continuum behavior which will also be described.

9:30 Determination of Sulfur in Organic Compounds by S₂ Emission

S. Shiffman and C. W. Frank, Dept. of Chemistry, University of Iowa, Iowa City, Iowa 52242.

This paper is concerned with the development of methods of determination of sulfur in organic compounds. A nitrogen-hydrogen diffusion flame is employed for the excitation of the S₂ band system after sample pre-treatment. Several continuous pre-treatment techniques involving on-line conversion of the sample enroute to the burner are discussed. The use of a column packed with carbon granules operated at a temperature of 750 °C is effective for reducing the structural dependence of S₂ emissivity for a number of organic compounds.

9:50 Coffee Break

Tuesday Morning (VI)

William G. Schrenk, Session Chairman, Dept. of Chemistry, Kansas State University, Manhattan, Kansas.

10:10 Interferences of Indium Chloride Emission in Low Temperature Flames

H. Liu and C. W. Frank, Dept. of Chemistry, University of Iowa, Iowa City, Iowa 52242.

Although the molecular emission method is sensitive, selective, and rapid for the determination

of halides, the most serious shortcoming of this method is that it suffers chemical interference effects from contaminant in the sample solution. This paper describes the effects of both cations and anions in the emission of indium chloride.

10:30 Trace Analyses with a Plasma Emission, Echelle Spectrophotometer

I. T. Urasa and R. K. Skogerboe, Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523.

The results of an evaluation of the capabilities of an echelle spectrometer coupled with an argon plasma for the determination of trace elements will be discussed.

10:50 The Development and Application of Television Direct Reading Spectrometry

J. D. Johnson, Spectrogram Corporation, 385 State Street, North Haven, Connecticut 06473.

The development of multichannel opto-electronic spectrometers is reviewed. Linear array devices are compared with echelle-image intensified TV systems. The successful development of an echelle-prism computerized direct reading spectrometer is described with emphasis on the interfacing of its several components. The system operates with conventional direct current arc sources and with a Cathaquant, a sputtering low pressure discharge source.

The applications of this system include copper based alloys, low alloy steels, and a number of plating and diffusion studies. Data are presented as intensity ratios against the least squares fit on the concentration of known standards. For in-depth compositional analysis, data are presented as intensity versus real time, which is then converted to concentration versus depth. Each real-time data point represents a depth of two to ten nanometres. Other wide ranging applications of the TVDRS system are discussed.

11:10 Precision and Detection Limits of Thorium and Uranium in Electron Probe Analysis

Robert H. Heidel, U.S. Geological Survey, Denver, Colorado 80225.

Precision and detection limits for thorium and uranium by electron probe analysis at 3σ confidence level are between 1500 and 2000 ppm for 20 kV-20 nA operating conditions for $M\alpha$ or $M\beta$ X-ray lines. Analysis is limited to use of M lines since no suitable crystals are available for the L wavelength range and also lack of homogeneous standard material of reliable composition.

11:30 Lunch

Tuesday Afternoon (VII)

Mrs. Pat Roberts, Session Chairman, Earth Sciences, Inc., Golden, Colorado.

1:15 Intermolecular Interactions in Various Transition Metal Hexafluoride Solids

Elliot R. Bernstein and *Gerald R. Meredith*, Chemistry Department, Colorado State University, Fort Collins, Colorado 80521.

The investigation of the low temperature near IR absorption spectra of ReF_6 in various isostructural MF_6 ($M = \text{Mo, W, Re, U}$) crystals and the investigation of the low temperature Raman spectra of various $M'\text{F}_6$ in MF_6 ($M', M = \text{Mo, W, Re, U}$) crystals have lead to several conclusions concerning:

- A) the importance of exchange in ReF_6 - ReF_6 interactions,
- B) the important contribution of the hosts to the molecular superexchange coupling mechanism,
- C) the magnitude of ground and excited state exchange interactions based on vibronic considerations,
- D) the contribution of two particle transitions to the vibronic structure,
- E) the magnitude and form of the interactions responsible for the appearance of two particle transitions.

These topics will be discussed in the presentation.

1:35 Laser Raman Spectroscopy in Water

Kirkwood M. Cunningham, University of Denver;
Marvin C. Goldberg, USGS, Denver, Colorado
80225; Eugene R. Weiner, University of Denver,
Denver, Colorado 80210.

Since the early 1930's, it has been realized that Raman spectroscopy is useful for the study of solutes in water, because of the relatively low intensity of the solvent bands. The advent of laser excitation, and the greater availability of high quality multiple monochromators and photon counting systems in the last decade has rendered this technique both more convenient to use and much more sensitive to highly dilute species in water. Therefore we have undertaken the first systematic evaluation of the sensitivity of Raman spectroscopy for the quantitative analysis of certain solutes which effect water quality. Although only laboratory methods have been made so far, our eventual goal is the development of a remote sensing device. With a total measurement time of 30 seconds, we were able to detect concentrations of 26 mg/litre for several dissolved anions in water.

1:55 Laser-Raman—An Infrared Spectroscopy of Higher Uronic Acids

Anthony T. Tu, N. D. Dinh, and C. Y. She,
Depts. of Biochemistry and Physics, Colorado State
University, Fort Collins, Colorado 80523.

Laser Raman spectra of hyaluronic acid, α -methyl-D-glucoside and β -methyl-D-glucoside were obtained before and after deuterium exchange. The differences observed in the spectra for hyaluronic acid and the two anomers were extensively analyzed. Among the several differences observed, the 842 cm^{-1} line was found to be the characteristic line for the α -anomer and the 890 cm^{-1} line for the β -anomer. It may be possible that these lines can be used for the identification of different types of glycosidic linkages in oligo- and polysaccharides. The 1279 cm^{-1} line is also a characteristic line for the α -anomer. Considerable differences in the spectra of —OH stretching vibrational modes indicate that the two anomers

have different types of hydrogen bonding. A very distinct line at 896 cm^{-1} and in the absence of the 840 cm^{-1} line indicates that hyaluronic acid contains only the β -glycosidic linkage. For further study, infrared spectra of hyaluronic acid were also investigated. Unlike monosaccharides, the hydrogen atoms in hyaluronic acid cannot be exchanged with deuterium. Both Raman and infrared spectra of hyaluronic acid indicated that they gave identical spectra before and after deuteration. This suggests that hyaluronic acid consists of some kind of helical structure and the water molecule cannot penetrate into the interior of the hyaluronic acid molecule.

This agrees fully with the X-ray diffraction study of hyaluronic acid by Atkins and Sheehan (1972) who found that hyaluronic acid consists of helical chains intertwining.

2:15 Atmospheric Attenuation of CO_2 Laser Radiation

S. S. R. Murty, EC31, Building 4487, NASA-Marshall Space Flight Center, Huntsville, Alabama 35812.

The $10.6\text{ }\mu\text{m}$ region of the atmospheric infrared window is not completely transparent due to the molecular absorption and scattering and the transmission of the laser radiation varies from line to line. The absorption coefficients due to the carbon dioxide, water vapor, and nitrous oxide are calculated from various pressures and temperatures of interest for atmospheric applications at several P lines. Application of the resulting data to the heterodyne laser Doppler measurements is discussed.

2:35 Coffee Break

Tuesday Afternoon (VIII)

N. Cyril Schieltz, Session Chairman, Professor Emeritus, Colorado School of Mines, Golden, Colorado.

2:55 Crystal Data for Some Iron Oxides of the Lanthanide Series

Ruth Botdorf, The Berks Campus of The Pennsylvania State University, R. D. 5, Tulpehocken Road, Reading, Pennsylvania 19608; Gregory

McCarthy, The Pennsylvania State University, University Park, Pennsylvania 16802.

Some oxides of the lanthanide series will combine with iron oxide to form complex oxides with the same structure as a group of naturally occurring silicates of certain divalent and trivalent metal oxides. The characteristic color of these crystals is green while those found in nature vary in color due to their composition.

These complex oxides were prepared by weighing stoichiometric amounts of the various oxides, grinding the mixtures, making pellets from the powdered material, and heating at a high temperature for one to two days. X-ray powder diffraction measurements were made with a diffractometer using nickel filtered copper K alpha radiation. From this information crystal data such as cell parameters, cell volume, and density have been calculated and refined with the use of a computer program.

The synthesized compounds have magnetic properties. In some instances compounds of similar structure have found many uses based on this property.

3:15 Trace Metal Techniques in X-Ray Fluorescence

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X-ray fluorescence has been utilized to determine trace metals in a variety of matrices applying a wide array of techniques. The procedures include both direct excitation of the "bulk" sample or excitation after preliminary isolation of the specific trace elements desired.

The following techniques have proven useful for trace metal analysis by X-ray fluorescence: (a) Ion-Exchange Papers; (b) Ion-Exchange Resins; (c) Filter Deposition; (d) Extraction-Adsorption; and (e) Chemical Co-precipitation ("COPREX"). Available applications of the above-mentioned procedures are surveyed inclusive with specific practical applications. The chemical co-precipitation procedure is described in detail, with selected applications in the areas of water pollution,

water analysis, metallurgy, and mineralogical samples. Specific precipitating agents used in conjunction with the "COPREX" procedure are reviewed from an application standpoint. Data are presented for the determination of the following elements: Ag, As, Ba, Bi, Cd, Co, Cr, Cu, Fe, Mn, Mo, Pb, Sb, Se, Sn, Ta, Ti, V, Y, and Zr.

3:35 Environmental and Clinical Application of Energy Dispersive X-Ray Fluorescence

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An energy dispersive X-ray system has been established and sample preparation techniques developed which permit rapid quantitative analysis of a wide variety of samples for 15 to 20 common metals which are generally considered to be either necessary for or toxic to human life. This system is finding wide commercial application for routine analysis of both environmental samples and clinical specimens. The environmental samples consist primarily of water, waste water, air filters, and gasoline. They are submitted by both governmental and private sources throughout the San Francisco Bay Area. Clinical specimens consisting of human hair, serum, and urine are submitted by medical doctors throughout the country who are pioneering in the field of preventative medicine. Data will be presented and interpretations will be discussed.

3:55 Differential and Isothermal Dehydration States of Retgersite ($\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$)

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Thermal dehydration of nickel sulfate hexahydrate monoclinic was studied by differential thermal analysis and oven drying. Reactions were determined by X-ray and chemical analysis. The dehydration of nickel sulfate is strongly influenced by experimental conditions as is the crystallinity of the various hydrates. The reason for this is not apparent and more work should be done on this subject. The pentahydrate occasionally reported in the literature was not formed in any of the experiments. Additional studies are necessary to see if such a hydrate exists.