Review: Infrared Spectrometry

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INTRODUCTION

This review covers mainly publications cited in *Chemical Abstracts*, volumes 92–95 (1980–81), through the December 28, 1981 issue (Jan. 11, 1982 issue of *CA Selects*).

Selection of References. The initial selection was based on *CA Selects: Infrared Spectrometry (Physicochemical Aspects)* and *Infrared Spectroscopy (Organic Aspects)*. *CA Selects* have proved to be a far more useful source for this review than *CA Search* which was used for the previous five reviews. The main advantage of *CA Selects* is that they contain complete abstracts rather than citations and keywords only. A disadvantage has been that *CA Selects* were not available to this reviewer in computer readable form like *CA Search*. However, most of the citations have been taken from the SDC *CA* database in computer readable form (*1*). The citations from SDC were parsed and rearranged into the standard citation form for *Analytical Chemistry* by computer. Thus, in a sense most of the bibliography of this review has been effectively keyed by *Chemical Abstracts* as has been the case for the three previous reviews.

This year, the review is again being submitted to *Analytical Chemistry* in computer readable form. A new version of the computer program *LISE (Literature Search and Edit)* which has been described in previous reviews was used to manipulate the citations.

The full *CAS* database for 1980–81 contains about 925,000 citations. The total number of citations on infrared by *CA Selects* was about 15,500, 10,000 in *Physical Aspects* and 5,500 in *Organic Aspects*. This is nearly twice the number reported in the review for 1978–79. A large proportion of the citations merely indicate a supporting role in the characterization of materials. Many arbitrary choices have been required to trim the remaining 3000 citations to the approximately 600 which make up the bibliography.

Books and Reviews have been selected to give broad coverage not only of infrared analysis, but also of other topics which provide support for analytical applications. The remaining papers have been selected with two points in mind: (1) to cover areas in which new developments are underway, and (2) to give broad coverage to applications of infrared to chemical analysis. Since infrared spectrometry is basically an instrumental technique, considerable attention has been paid to instrumental developments.

This review has a strong bias toward papers in English. Since Russian and Japanese journals are difficult for the readers of *Analytical Chemistry* to obtain and to read, a condition for inclusion of citations to papers in these languages is that *Chemical Abstracts* contain a useful, if brief, description of the work. This has eliminated a number of interesting titles. Because of the bias introduced in this way, the reader is cautioned against judging the activity in different countries by a citation count.

Organization of the Bibliography. Books (*A*) and Reviews (*B*) contain those citations which were so classified by *Chemical Abstracts*. The remainder of the bibliography is divided into seven main sections according to subject matter, and these are divided into subsections. The text of the review is also divided into parallel sections and subsections. Each section amd subsection of the bibliography has separate numbering distinguished by literal prefixes. Prefixes for main sections are single letters; those for subsections are double letters with the first corresponding to that for the main section to which the subsection belongs. These sections contain only citations to current papers. Any citations to older papers, to oral presentations, etc., are in a separate footnote section whose entries are numbered without the literal prefix.

CA abstract numbers are included for most citations to facilitate location of abstracts when journals are not readily available. Abstract numbers for books are omitted because the abstracts generally contain no additional information beyond the citation. In the case of reviews, only a few of the abstracts contain information on subject matter, but most contain only the numbers of references (which are also included in this Bibliography).

The citations for books have been sorted alphabetically by title. Those for reviews have been sorted alphabetically by journal citation to facilitate looking up the original reviews. Citations for all other sections have been sorted by *CA* abstract numbers with the most recent appearing first.

Each citation in the bibliography contains the complete title in English as given by *CA*. Inclusion of the titles follows a strong personal conviction of this reviewer that the title is an integral part of any bibliographic citation. The titles are effectively part of the text and must be scanned to get the full message of this review. Each citation starts with the title to facilitate scanning by the reader.

The abbreviation, *ibid*, has not been used. Each citation is complete and can be clipped and pasted on a card if desired.

GENERAL TRENDS IN ANALYTICAL INFRARED SPECTROMETRY

Scope of Infrared Spectrometry. The overall scope of infrared spectrometry (spectroscopy) has been well summarized by Dr. A. Lee Smith: (*2*)

"Infrared spectroscopy is used by workers in many disciplines, but the term carries a different meaning in each field. To the analytical chemist, it is a convenient tool for solving problems such as determination of the five isomers of hexachlorobenzene, characterization of the wax, resin, polymer, and emulsifier in emulsion polishes, and identification of the country of origin of illegal opium. To the physicist, it may represent a method for studying energy levels in semiconductors, determining interatomic distances in molecules, and measuring the temperature of rocket flames. To the organic chemist, it furnishes a way of fingerprinting organic compounds, picking out functional groups in an organic molecule, and following the progress of a reaction. To the biologist, it promises a method of studying transport of bioactive materials in living tissue, provides a key to the structure of many natural antibiotics, and gives many clues in the study of cell structure. To the physical chemist, it can furnish a revealing look at mechanism of heterogeneous catalysis, provide a convenient means for following the kinetics of complicated reactions, and serve as an aid to determining crystal structures. In these fields and many others, infrared spectroscopy provides researchers with powerful insights. It is probably fair to say that infrared is the most nearly universally useful of all instrumental techniques."

Strengths and Weaknesses. We now review the strengths which make infrared spectrometry so widely applicable and outline some of the problem areas, many of which are being attacked by new techniques and instrumentation discussed by papers cited in the bibliography.

The major strength of infrared spectrometry is applicability to both qualitative and quantitative determination of chemical functionality of a wide variety of covalent bonded chemical substances, including gases, liquids, polymers, and solids, both crystalline and amorphous.

Widely available spectrometers can produce a high quality infrared spectrum in less than five minutes. The instruments are easy to use, and many university and industrial laboratories provide staff or students with self-service spectrometers which are available around the clock. The availability and short turn-around time thus afforded are important factors in a chemist's productivity. Cost of such a machine is comparable with that of his secretary's word processing machine.

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The infrared spectrum of a substance is a mapping of its internal vibrations, i. e., the spectral data consists of vibration frequencies and intensities of interaction with infrared radiation. A great deal can be determined about the nature of a substance by off–hand examination of its spectrum. Presence of various types of atoms or bonds or functional groups or other structures is inferred by comparison with a large body of empirical correlations which have been built up over many years. Frequencies and intensities are sensitive to local structure, orientation, physical state, conformation, temperature, pressure, and concentration. It is this sensitivity combined with the chemist's knowledge of the system which makes the technique so useful. However, because the spectral features tend to overlap, interpretation is often somewhat fuzzy and supplemental information is required for a firm identification.

On the one hand, the spectrum can serve as a fingerprint to check the identity of a reactant, product, or intermediate by matching against known reference spectra. On the other hand, the various spectral features can be used to characterize the chemical functionality of substances for which reference spectra are unavailable. It is rare to be able to explain every feature of a spectrum or to make a complete structure proof even of a pure compound on the basis of its infrared spectrum alone. Interpretation of spectra is a skilled art, but one which is part of the repertoire of a growing number of chemists. Interpretation and matching of spectra by computer is an active area of research but as yet it is no match for the capability of a skilled chemist.

Infrared spectrometry is a technique of intermediate sensitivity. Intensities of major absorption bands of most substances lie in the same range (100–1000 cm^{-1}) for condensed phases. It is rare to find a strong band which is 1000 times as strong as its immediate surroundings. For most pure substances, half a dozen or more well defined absorption bands can be measured accurately enough to give a definitive identification on a smear or film less than a thousandth of an inch thick and a few millimeters in diameter. Generally, the spectrum provides information on components which are present in percentage amounts in relatively simple mixtures. Extensive calibration or chemical or physical separations may be required for analyzing multicomponent mixtures, especially when the minor components are of interest. Special techniques and favorable circumstances are required for extreme sensitivity in the ppm or ppb range.

Infrared *absorption* is the property of interest, but it is rarely measured directly. Most spectrometers determine the *transmission* of a sample. Because of the exponential nature of the absorption law, concentrations are actually proportional to the difference between the logarithms of incident and transmitted radiation. Serious problems arise for weak absorption bands for which the absorbance is a small difference between two large quantities. For strong absorption bands there are problems due to the nature of the logarithmic function itself. The S/N of dispersion and Fourier spectrometers tends to be independent of the of the specimen. Thus, an instrumental S/N of 1000:1 in transmission corresponds to a S/N of 100:1 in concentration at an absorbance of 1, 10:1 at an absorbance of 2, and 1:1 at an absorbance of 3. For tunable lasers, the situation is more favorable because the S/N tends to be proportional to the transmitted signal. Although tunable lasers permit measurements up to about an absorbance of 5, extension of the high absorbance range is clearly in the direction of decreasing returns. Expansion of the low absorbance range has the advantage that the function is linear, but means must be found to measure absorbance directly and avoid measuring it as the difference between large quantities.

In laboratory chemical analysis, the interplay between infrared, Raman, NMR, and mass spectrometry, as well as ESCA and other techniques for determining chemical functionality is very important. Of the major instruments for determining chemical functionality, the infrared spectrometer is the least expensive and easiest to use. Hence, it tends to be the choice of smaller laboratories with limited budgets. Infrared equipment is more portable, and probably is applicable to a wider range of practical problems. However, for larger laboratories which can afford several, or even all of these techniques, there are choices to be made when it comes to performing analyses. Where modern, high field NMR capability for ^{13}C is available, infrared may not be the first choice for liquids and soluble solids. Where modern, high resolution GC–MS is available, infrared may not be the choice for analysis of complex multicomponent mixtures which require capillary GC columns for separations. Where modern Raman equipment is available, infrared may not be the choice for measurements on water solutions. Where modern ESCA equipment is available, infrared may not to be the choice for studying the chemistry of the first 10–50 A of a surface layer. On the other hand, where in–situ measurements of a substance or rapidly changing flowing stream are required, infrared is likely to be the choice.

In the real world of the control lab and plant process control, infrared is used far more than any of the other techniques mentioned in the previous paragraph. There, the choice must usually be made between a chromatographic separation technique and infrared. Infrared tends to be better for simple mixtures and continuous measurement while chromatography tends to be better for complex mixtures which do not require rapid response.

Trends in Infrared Spectrometry. There has never been a time when so many talented people have been working so effectively to expand the capabilities of infrared spectrometry.

As everyone knows, the most dramatic trend in infrared spectrometry is in the direction of computerization of all aspects of acquisition, processing and storage of data, as well as identification of spectra. The computers have not yet taken over sample preparation, but they make it easier to obtain useful spectra from less than optimum samples.

Increasingly spectrometers put out spectra in digital form which is transportable and storable *error free*. Presently, JCAMP is organizing a program for standardizing the interchange of such digital spectra between users of spectrometers of diverse origin. There is need for means for publishing, or at least archiving such data with public access. When the effort has been expended to prepare, purify, and record the spectrum of a rare or unstable compound, the data should be made available to the scientific community at large without loss of accuracy. And this is technically feasible at the present time.

Fourier spectrometers are becoming much cheaper, but they have not yet matched the cost of the intermediate dispersion spectrometers. For routine laboratory qualitative scans, the Fourier and dispersive spectrometers seem more or less equivalent. A complete spectrum can be acquired and plotted with either in about two minutes. Older dispersive spectrometers were subject to tracking errors when run at this speed, but with microcomputer control this is no longer the case. The Fourier spectrometer can actually acquire the interferogram two orders of magnitude faster than this. The rate limiting steps are transforming the data, and plotting it. Even as this is written, high speed array processors and hard wired FFT processors are being employed to speed up the

calculations, and in the opinion of this reviewer, it is only a matter of time until the Fourier transform is routinely processed in near real-time.

Dispersive spectrometers do not compete effectively with Fourier spectrometers for measuring time dependent phenomena with time constants from a few seconds to a minute when the whole spectrum is needed, i.e., on-line LC, GC, evolved gas analysis, and polymer relaxation studies. For single wavelength measurements at rates faster than the scan time of the Fourier spectrometer, the dispersion machine is more effective, but it is likely to be competing with a laser spectrometer.

Laser spectrometry is a really exciting development which is now unfolding. The properties of laser spectrometers include ultra high intensity, ultra high resolution, and very high spectral purity, together with a small highly collimated beam and often a very rapid scan rate, everything the spectroscopist has always wanted. At the present, the major shortcoming of commercially available systems, mainly tunable diode lasers (TDL's), is their very narrow tuning range, of the order of 1 cm^{-1}. This is not enough to scan across even a very sharp band of a solid, but it can do wonders with the sharp lines of low molecular weight gases. Laser spectrometers cited in the bibliography are claimed to cover the entire range of the usual grating or Fourier spectrometer, but this reviewer is not familiar with any which can scan the standard region from 4000 to 400 cm^{-1} routinely in a few minutes. When such spectrometers will be available to chemists for routine analysis is anyone's guess. They will make many new applications feasible, but it will be hard to match the multiplex capability of the Fourier spectrometer for routine acquisition of complete spectra.

Computer data processing has received a great stimulus from the Fourier machines. Their powerful minicomputers have provided opportunities for many different techniques for enhancing spectra by processing in the Fourier domain rather than the spectral domain. This is an area which every serious spectroscopist needs to understand. These techniques are applicable to spectra from dispersion spectrometers as well, but this reviewer is of the impression that computer power of such systems is marginal for these computations. As the value of such calculations is appreciated, the data processing power will undoubtedly increase.

Computer identification of spectra is a rapidly growing area. There are two major aspects to this activity, search and match, and interpretation. Most commercially available data systems have one or both. The search database is a compromise between number of compounds and completeness of representation of spectra. It seems clear at this time that the more complete the spectra, the better the matching capability.

The cost of building a library of digital spectra is astronomical even though the spectrometer carries out all of the digitization. The number of systems in the field which can make use of such libraries is increasing rapidly and may well support the cost if suitable means can be provided for the user to have his own search file. Video disks may be the answer.

Use of FT-IR in combination with chromatography is another area of rapid growth. Sensitivity has improved to the point that WCOT and capillary columns can be used quite effectively.

Photoacoustic spectroscopy is a very exciting new sampling technique which is discussed at length later in this review. Its main advantages are that it simplifies sample preparation for solids to practically no preparation at all and it measures radiation *absorbed* by the sample, not what passes through it. However, for the present, somewhat longer times are required to obtain the same S/N as by conventional techniques. Additionally, there are questions about applicability to quantitative analysis.

(A) BOOKS

Several books are rich sources of review articles on various aspects of infrared spectroscopy: (*A2*), (*A3*), (*A4*), (*A5*), (*A22*), (*A26*), (*A31*). For those books which consist of separately authored chapters, the individual papers which fall within the scope of this review are also cited separately under Reviews.

Nearly half of the books consist of collections of spectra: (*A7*), (*A9*), (*A10*), (*A11*), (*A15*), (*A18*), (*A19*), (*A20*), (*A28*), (*A29*), (*A30*), (*A8*). The trend is toward comprehensive sets of spectra in relatively large books or sets of books. This is encouraging because it brings the cost of a reasonably useful collection of spectra within the reach of the individual user of infrared. Two groups are independently producing systematic sets of atlases of high quality spectra covering a wide range of compounds: Sadtler Laboratories (*A28*), (*A30*), (*A8*), and the Coblentz Society (*A18*), (*A19*), (*A15*). In both cases, the spectra have been selected from large collections which are available on microfilm or microfiche, but which are too large and too expensive for small laboratories and individuals. All of the spectra in these atlases are plotted as transmittance vs. wavenumber.

The second of the three part set of the *Hummel-Scholl Atlas of Polymer and Plastics Analysis, Vol. 3. Additives and Processing* Aids, has appeared (*A9*). The 6708 spectra are indexed by chemical name and by empirical formula.

The second edition of *An Infrared Spectroscopy Atlas for the Coatings Industry* has grown to enormous size (*A7*). This book attempts to cover in one volume what Hummel-Scholl covers in three. Spectra are ordered according to chemical type. There is no index to permit them to be located by chemical name, but they are indexed by trade name or by manufacturer. The book also contains a comprehensive bibliography of papers on polymer spectra which is indexed according to chemical type.

The third edition of *The Aldrich Library of Infrared Spectra* has also appeared (*A29*). This edition contains a full 12000 spectra and rivals the size of an unabridged dictionary. This is the most comprehensive single volume of spectra presently available, and the cost is such that the individual chemist can afford a personal copy. Spectra are organized according to chemical functionality. The book contains empirical formula as well as chemical name indices, and is cross indexed with the Aldrich Chemical catalog, and vice versa. The format of 16 spectra per double page facilitates cross comparison of spectra of related compounds. However, size of the book makes it awkward to xerox individual spectra. The spectra are plotted with abscissa linear in wavelength, with a non-linear frequency scale along the top of the charts. This is a drawback for users who are accustomed to spectra which are plotted linear in frequency as in other collections mentioned above.

Three books devoted mainly to FT-IR spectroscopy have appeared since the last review of this series. The first, *Infrared Interferometric Spectroscopy* by Martin (*A9*), is a review of the theoretical background of FT spectroscopy, with brief descriptions of instruments which are now available. Polarization effects and methods for measuring refractive index are discussed. The second, *Spectrometric Techniques*, edited by Vanasse (*A26*), contains three papers on specific aspects of the technique of Fourier spectroscopy with an up-to-date review of tunable IR tunable laser spectroscopy in addition. The third, one of the NATO Advanced Study Series edited by Durig (*A22*), contains some 26 papers on a broad range of topics having to do with applications of FT-IR to analytical problems, and for this reason, it is probably of more interest to infrared analysts than the other two.

Bellamy's *Advances in Infrared Group Frequencies* has appeared as a second edition ten years after the first. Approximately one third of the book has been rewritten. This is now regarded as Volume 2 of *The Infrared Spectra of Complex Molecules*. Volume 1 is primarily concerned with the experimental observations of group frequencies while the present volume is primarily concerned with explaining *why* group frequencies are dependent on changes in chemical structure. As Bellamy points out, "One cannot interpret an infrared spectrum without a good knowledge of the experimental facts, but too rigid an interpretation without any understanding of how the facts originate can lead to gross errors".

Two up-to-date books have appeared on vibrational spectroscopy as applied to surfaces. The first is *Vibrational Spectroscopy of Adsorbates* (*A32*), edited by Willis, and the second is *Vibrational Spectroscopies for Adsorbed Species* (*A2*), edited by Bell and Hair. Both of these books cover other techniques as well as infrared spectroscopy for measuring the vibrational spectra of surfaces, including inelastic tunneling spectroscopy (IETS), surface enhanced Raman spectroscopy (SERS), electron energy loss spectroscopy (EELS), etc.

(B) REVIEWS

The number and wide range of the included reviews precludes even a cursory mention of each. In most cases, the title gives enough indication of the subject matter so that additional comments do not seem necessary. Some estimate of the comprehensiveness of a review can be obtained from the length and number of references, both of which are given in the bibliography.

For the most part, individual reviews will be cited in the appropriate section which follows. However, there are a number of reviews of interest which do not fall under any of the classifications. Numerous reviews have appeared on group frequencies (*B6*), (*B10*), (*B47*), (*B68*), (*B79*), (*B93*), *B-(119–133)*, (*B142*), and (*B150*). Matrix isolation has received considerable attention also (*B8*), (*B74*), (*B88–B92*). Applications of infrared spectrometry to astronomy have been reviewed (*B16*), (*B39*), (*B100*), (*B117*), as well as to hydrogen bonding and molecular association (*B56*), (*B65*), (*B66*), (*B89*), (*B136*), (*B143*), and to the solid state (*B45*), (*B62*), (*B63*), (*B83*), (*B84*), (*B103*), (*B116*).

(C) ANALYTICAL APPLICATIONS

Use of infrared spectrometry for all types of analytical applications is continuing to expand. It is used for quality control of incoming and outgoing products, for problem solving, for examining competitor's products, for monitoring laboratory reactions, for process monitoring and control, and others. It is not possible to cover this field adequately in the time and space for this review. Actually, most of the techniques and many of the applications have been described in the literature long ago. We note here mainly areas in which activity has increased dramatically in the last few years (near infrared reflectance, semiconductor and coal analyses, gas analyses by tunable diode lasers, etc.) or which seem notable for other reasons (process monitoring, electrode reactions, studies of time dependent phenomena, etc.). Numerous reviews have been published on topics relevant to chemical analysis (*B1*), (*B26*), (*B36*), (*B37*), (*B76*), (*B79*), (*B138*).

Determination of oxygen to 10^{-4}% in high purity selenium using the 932 cm^{-1} band has been reported (*C1*). An IR spectrometric method has been described for quantifying soot in piston deposits, crankcase oil insolubles, or directly in the oil of diesel engines (*C2*). An IR method for monitoring the neutralization of corrosive acids in engine oil is claimed to be more meaningful than the classical TAN/TBN titrations (*C3*). A method has been reported for determining the ethanol content of any type of gasoline using the 880 cm^{-1} band which is absent from the spectrum of other alcohols (*C4*). A system has been described for continuous monitoring of methane evolved from soil and water which has a sensitivity of 0.01 ppm. with a response time of 1 s. This enables determination of fluxes of the order of 10^{-4} g/m^2 per day in under 20 minutes (*C5*). IR determination of cyanogen in organic solvents has been standardized using base catalyzed disproportionation to CN^- and CNO^-, followed by potentiometric titration (*C9*).

Time dependence of the alcohol content of breath has been studied with the Alcotest IR 7010 (*C8*). Tracer gases, CO_2, N_2O, and SF_6, have been used to determine ventilation rates and spreading routes in the workplace. Continuous monitoring of N_2O with an IR spectrophotometer was the most practical (*C10*). A 20 meter multiple pass gas cell and IR spectrophotometer have been used for quantitative trace analysis of operating room air pollutants (*C13*). An IR gas analyzer has been used to monitor the operation of carbon beds for adsorption of organic vapors (*C16*).

Medical use of IR for determination of slight enrichment of D_2O in physiological fluids has been described (*C17*). IR quality control of incoming materials, indentification and quality control of textile finishes, and fiber identification in a textile mill has been described (*C19*). FT-IR has been used to detect transfer of silicone release agent to composite surfaces during fabrication (*C22*).

(CA) Near Infrared Reflectance. Osborne has reviewed principles and practice of near infrared reflectance analysis (*B42*). Use of near infrared diffuse reflectance for determination of protein, fat, and moisture in grain, milk, meat and other natural products is expanding. This region, from 1 to 2.5 micrometers, contains mainly overtones and combinations of hydrogen vibrations of OH, NH, and CH groups. Highly precise diffuse reflectance values for a number of wavelengths are measured, often directly on grain without pretreatment. However, there are indications that finer particles are preferable. Calibration is carried out by multiple regression analysis of data for a very large number of known (chemically analyzed) samples which bracket the analytical range. The absorption bands overlap so badly that the average spectroscopist would not believe that the method could work. However, reproducibility is comparable with that of chemical methods. The time for a determination is of the order of a few minutes. Success is undoubtedly dependent on the uniformity of the composition of natural products. It seems likely that variations of this method can be used for analyzing other organic powders, pellets, and possibly inorganics, especially for water of hydration. The method appears to have promise for process control of granular solids. Transmittance can be used for materials which do not scatter radiation too badly.

Near-IR reflectance data on whole wheat kernels have been analyzed by stepwise multiple linear regression to select wavelengths for protein determination (*CA1*). Moisture and α-acid content of hops have been determined simultaneously by near IR reflectance with about 1 min analysis time (*CA5*). Near IR reflectance gave comparable accuracy with standard techniques for 89 samples of rapeseed kernels. Values for glucosinolate and chlorophyll content were less satisfactory (*CA3*). Near IR has been reported to be suitable for rapid determination of lysine and nitrogen for plant breeding programs to improve lysine content of barley proteins (*CA16*).

Accuracy of near IR reflectance for determining fat, protein, and moisture in fresh meat has been evaluated (*CA7*). Feasibility of determining composition of wheat, soybean, pork and fresh potatoes with two types of NIR instrument has been studied (*CA8*).

Higher accuracy has been claimed for near-IR determination of fat, nitrogen, and lactose than for standard methods (Rose-Gotlieb for fat, Kjeldahl for nitrogen, and gravimetric for lactose) (*CA11*). Performance specifications for infrared milk analyzers have been discussed in detail (*CA14*). Errors in estimation of fat, protein, and lactose in milk have been evaluated for the Multispec instrument (*CA15*).

Near IR reflectance has been evaluated for determining fructose, glucose, and sucrose in model systems intended to represent major constituents of dried apple tissue (*CA10*). Bound water and excluded volume for proteins in aqueous solution have been determined by near IR difference spectra (*CA17*).

(CB) Surface Applications. The term surface means different things to different chemists. To the physical chemist it probably means a region of a few monolayers thickness. To the organic chemist, it probably means a region of a few microns thickness which is important for coatings of various kinds. In this section, it is the former definition which applies. Information on thicker surface layers is considered in section (*HF*) on internal reflection.

Since the absorbance of the strongest of infrared bands is no greater than unity for a sample thickness of about one micron, measurements at the monolayer level are difficult.

The most popular techniques for measuring the spectra of surface functional groups are transmission and diffuse reflection, for high area powders, and specular reflection at a high angle of incidence, for smooth metal surfaces. Several hundred papers in these areas alone have appeared since the last review. Two books specializing on vibrational spectra related to surfaces have appeared, one edited by Bell and Hair (*A2*), and the other by Willis (*A32*). A number of reviews on surface applications have appeared (*B2*), (*B3*), (*B4*), (*B28*), (*B49*), (*B80*), (*B109*), (*B131*), (*B134*), (*B140*), (*B146*).

The surface groups of aerosil silica are by far the easiest to study. Even in this case, quantitation is difficult. Quantitative determination of surface bound groups, especially isolated silanol groups on SiO_2 particles by IR spectroscopy has been described (*CB11*). Transformation of SiCl and $SiCl_2$ groups into NH_2 groups by reaction with NH_3, and transformation of $SiNH_2$ groups into SiOH groups by hydrolyzing with small doses of water has been studied by IR spectroscopy (*CB1*). The method is also applied to catalytic metals supported on high area substrates. IR has been used for monitoring CO chemisorption on a Pd/SiO_2 catalyst under flowing conditions between room temperature and 200°C (*CB3*).

Specular reflection techniques are relatively difficult. Commercial spectrometers usually must be modified for such work. Design and operation of instrumentation for IR reflection–absorption spectra from 10^{-11} to 10^{2} torr and from 77 to 1200K has been described by Golden and Overend. The technique can detect vibrational spectra at submonolayer coverage on low area surfaces (*CB2*). Adsorbed molecules have been detected by measuring temperature changes due to absorption of IR radiation by CO adsorbed on evaporated Ni while spectra were measured by rapid-scan FT-IR. Spectra are shown for a range of CO coverages on an evaporated Ni film and on a film damaged by ion bombardment (*CB5*). IR ellipsometric spectroscopy (IRES) has distinguished CO in a variety of surface structures on Ni (100) (*CB7*). FT-IR has been used to study adsorbed HOAc and 2,4-pentanedione on oxide covered Cu and Al (*CB8*).

Liquid interfaces have been difficult to study because it is not easy to obtain a high enough ratio of surface to bulk absorption. FT-IR study of aqueous Na *n*-hexanoate has given information on progressive aggregation and Na ion binding with increasing concentration (*CB9*). IR studies have been reported on ion exchange of carbon films in solutions of $NaHCO_3$, Na_2CO_3, and NaOH (*CB12*).

Reactions between an evaporated Fe film (500–1000A) and lauric acid/dodecane have been studied by transmission IR spectroscopy with a heated high pressure diamond cell (*CB10*). Adsorption of macromolecular materials on Ge from a dilute bacterial (*Flexibacter*) culture in artificial seawater has been studied by ATR IR spectrophotometry (*CB13*).

(CC) Semiconductor Applications. Hundreds of papers have appeared in the past two years on use of infrared for measuring various properties of semiconductors, mainly silicon. For electrically active impurities or dopants like boron and phosphorus, the required sensitivities are of the order of a few ppb. This is well beyond the capability of measurement by *vibrational* absorption bands. However, intensities of absorption bands associated with the excitation of charge carriers (electrons or holes) are orders of magnitude greater than for vibrational absorption bands. Silicon shows absorption lines due to hydrogen-like spectra of bound electrons and holes in the 300 cm^{-1} region which permit differentiation between different electrically active impurities in the ppb range. It is necessary to cool samples to helium temperature to bind the charge carriers.

IR methods for determining foreign atoms in Si crystals are faster, and usually more informative, than electrical methods. Some FTIR artifacts which could be misleading have been noted (*CC14*). Detection limits in the high ppt range are feasible by absorption techniques using FT-IR (*CC10*). This is not the only technique which can achieve these sensitivities. Simultaneous determination of boron and phosphorus in Si crystals has been achieved by a photoluminescence method using calibration standards prepared by neutron–transmutation doping and vacuum multipass float-zone techniques (*CC2*).

Oxygen and carbon impurities in silicon are usually determined by infrared measurement on vibrational absorption bands at 900 and 607 cm^{-1}, respectively. The sensitivity requirements are not quite as great as for electrically active impurities. Absorption of oxygen increases, and lattice absorption decreases in silicon down to about 78°K, but considering measurement time, specimen size, and cost, room temperature measurement is claimed to be more advantageous (*CC12*). Determination of both C and O in single crystal silicon at concentrations of ~0.1 ppm in measurement times of ~1 min is claimed for FTIR combined with subtraction relative to a pure reference wafer (*CC13*). A rapid, precise, and sensitive method for determination of C and O in single crystal Si is claimed to be an improvement of the standard ASTM method due to the characteristics of FTIR instrumentation (*CC15*). Concentration profiles of interstitial O have been obtained by scanning IR absorption in Si crystals (*CC8*).

Presently there is considerable interest in ion implantation of silicon with nitrogen, oxygen, and other atoms. Dosage is very high, and all of the implanted atoms stop within a few micrometers of the surface. For nitrogen, the concentration of implanted atoms can be high enough to exceed the stoichiometric amount for Si_3N_4 in a very thin layer under the surface. When the damage is annealed, either by laser bombardment or heating, an insulating layer of Si_3N_4 is formed a few microns below the surface. Spectra of single crystal Si implanted with ~10^{18}/cm^2 N ions show fringes by interference of radiation reflected from the front surface and the buried layers. Detailed theoretical analysis provides information on the range and straggling of implanted ions (*CC9*).

Another area of high activity in infrared analysis is that of amorphous Si and Si/hydrogen alloys and related materials, mainly for solar cells. FTIR has been used to observe hydrogen incorporated in grain boundaries and on the surface of solar-cell polycrystalline Si exposed to rf- and d.c.-induced hydrogen plasmas (*CC1*). IR band frequencies of oxygenated polysilane samples correspond with bands that arise during exposure of hydrogenated α-Si films to air (*CC3*).

IR has also been applied to study of the mechanism of deposition of silicon from silicon tetrachloride. Gas phase components such as $SiCl_4$, $SiHCl_3$, SiH_2Cl_2, HCl, $SiCl_3$, and $SiCl_2$ have been observed by in-situ IR in the epitaxy from $SiCl_4$ and H_2 at high temperatures (*CC4*).

At the other end of the concentration scale, IR has been used for measuring carrier concentrations. Calibration curves have been reported for measurement of carrier concentration in Si and GaAs from the wavelength of reflectivity minima (*CC5*). IR reflection and transmission spectra have been used to determine carrier concentrations of 10^{19} to 10^{20} per cm^3 in polysilicon layers deposited by low-pressure chemical vapor deposition on oxidized Si substrates (*CC6*).

(CD) Coal Analyses. Another field of high activity is the use of IR to investigate coal and processes for gasifying coal. Use of FT-IR to study organic structures and inorganic components of coal has been reviewed by Painter and Coleman (*B12*). The problems associated with application of FT-IR to characterization of coal structure have been critically discussed (*CD1*). The distribution of vacuum devolatilization products of 12 bituminous coals and a lignite have been determined by FT-IR (*CD2*). Absorption bands present in spectra of pyridine and Me_2SO extracts and residues provide information on the nature of coals which can be correlated with their combustion process (*CD4*), (*CD7*).

One of the serious problems in storing coal is that some coals tend to heat spontaneously. FT-IR has been used to investigate samples from a test pile of bituminous coal which was subject to spontaneous heating (*CD8*).

(CE) Forensic Applications. Kubler has reviewed the possibilities of GC/IR in forensic science (*B22*), and Ganschow and Heil have reviewed use of IR in drug control (*B50*).

It came as a surprise to this reviewer that enough of a volatile accelerant like a low boiling petroleum fraction remains at the origin of a fire to allow it to be identified. Accelerants from arson debris have been concentrated by a gas purging/adsorption elution technique followed by gas chromatography and IR spectroscopy (*CE4*).

The use of paint analyses for identification is much better known. A forensic method based on comparison of differences in absorbance of selected band pairs has been described for paint analysis (*CE2*). IR spectroscopy was used to establish a data base from 254 samples of automotive refinishing products for comparison with spectra of unknown samples (*CE5*).

(CF) Electrolytic Studies. Reviews by Bewick (*B34*), Waters (*B58*), Symons (*B112*), and Badiali (*B113*) have appeared on topics related to IR and electrode chemistry. A relatively new area for IR is in the study of electrode processes. The use of semi-transparent evaporated electrodes on ATR crystals as electrodes permits the active surface to be observed through the metal film. FT-IR was applied to detection of products at the surface of evaporated Fe electrodes on a 45° Ge ATR crystal during slow potential scans (*CF3*). More recently, the electrode/electrolyte interface has been studied by reflection from the electrolyte side, transmitting the radiation in and out through a very thin layer of electrolyte. This and other related techniques have been reviewed by Bewick, Fleischmann, and Robinson (*B34*).

One of the intriguing aspects of studying electrode surfaces by IR is that the surface can be varied in-situ by scanning the voltage without disturbing the experimental arrangement. (*CF3*) (*CF1*).

(CG) Laser Applications. Tunable diode lasers offer most interesting possibilities. The unique characteristics of tunable diode lasers are ultra high resolution and very high intensity. They can also be scanned over a narrow wavelength interval

very rapidly. They are finding many practical applications in atmospheric and gas monitoring where their high resolution capability is essential, and also in process monitoring where high intensity and spectral purity provide increased dynamic range. Linearity of Beer's law plots has been demonstrated up to an absorbance of 5 (*CG6*). Their main drawback, aside from cost, is the narrowness of the free spectral tuning range. Actually, two frequency ranges need to be specified for current TDL's. The first is the broad range of 100–200 cm^{-1} over which they can be temperature tuned. The second, narrower range is approximately 1 cm^{-1} wide, not wide enough to scan even an unusually narrow band of a condensed phase sample. However, within this range electrical tuning at very high speed is feasible and the frequency can be controlled well enough to make reliable measurements on the side of a sharp band of a solid. Doppler broadening is the resolution limiting factor for measurements on gases at atmospheric pressure. It is routinely feasible to measure the intensity of a line of a minor gaseous component between the lines of a major gaseous component, for example, natural abundance and below of $^{14}CO_2$ in $^{12}CO_2$. A feasibility study on use of a tunable diode laser to perform radiocarbon dating has reported detection of ^{14}CO at concentrations of $^{14}C/^{12}C$ below 10^{-12}. Sensitivity is comparable to that of an ideal disintegration counter. Extrapolating to long time constants, it appears that carbon samples of a few hundred milligrams can be dated (*C6*).

The general field of tunable lasers, including those which depend on various non-linear optical effects, has been reviewed by Schlossberg (*B118*). This, and the following sections are limited to discussion of TDL's which have achieved much wider popularity than other lasers because of commercial availability. However, many of the interesting properties of TDL's are possessed by other lasers which have considerably broader tuning ranges. These are discussed mainly in the section on laser spectrometers.

Hydroxyl compounds have been determined in various solvents, and D_2O in H_2O, serum, and urine using a tunable diode laser at 1350 nm. Measurements can be made even on the edge of an absorption line (*CG1*). Bolometric detection of IR spectra has been accomplished by shining a TDL on a supersonic molecular beam used to study rotational distribution of CO in free jets (*CG4*). Local values for density and temperature of 2-dimensional flows of SF_6 and C_6F_{14} have been determined using discrete wavelengths from a CO_2 laser (*CG5*).

Several applications which make use of the large dynamic range have been reported. A very accurate value for the absorption coefficient of liquid water, 123±1.8, has been determined at 2950 cm^{-1} using a TDL spectrometer (*CG3*). A digitally controlled Pb salt tunable laser has been described for determining the residual concentration of $MeSi(OAc)_3$ in silicone rubber. The analytical wavelength was 30 cm^{-1} off the carbonyl peak to accomodate a reasonably thick flow-thru cell (*CG6*). Even in sooting C_2H_2–air flames, fully resolved profiles of one or more CO lines have been determined using a TDL (*CG7*).

(CH) Trace Gas Analysis. Because of the small diameter and high intensity of the TDL beam, multiple pass cells of considerable length can be used for trace gas analysis. Good S/N for measurement of 108 ppm of CO in a 10 cm path has been reported for a 2nd derivative, dual beam TDL spectrometer (*CH1*). A TDL derivative spectrometer coupled with a multipass cell has been used to determine a value of 298±5 ppb for the tropospheric N_2O concentration (*CH2*). Very high detection sensitivity for weak absorption lines of CO_2 has been reported for a TDL spectrometer using a 100-m multipass cell (*CH3*). Sensitivity of better than 100 ppt has been reported for a TDL spectrometer coupled with a 1-m multipass cell (*CH4*).

(CI) Automotive Exhaust Analysis. Time response for TDL measurement of CO (<25 ms) is fast enough to be useful in analysis of engine and emission control system dynamics (*CI1*). An IR analyzer using a Pb salt laser of improved design was able to detect minor oscillations in emissions of CH_4, CO, NH_3, SO_x, and NO_x (*CI2*). Use of TDL absorption spectroscopy for in situ determination of concentrations of species present in combustion flows has been discussed (*CI3*). TDL spectroscopy selectively determines CO in the presence of large amounts of water vapor, permitting the direct analysis of the full exhaust flow (*CI4*).

(CJ) Free Radical Spectra. The ν_2 = 1←0, 2←1, and 3←2 bands of methyl radical have been observed in the gas phase at 606.4531, 681.6369, and 731.0757 cm^{-1} by TDL spectroscopy (*CJ1*). IR microwave double resonance has been used to determine rotational, distortion, fine, and hyperfine constants for a number of rotational states of isotopic species of ClO_2 (*CJ2*). High resolution TDL IR spectra of the Cl atom, NF_2, CF_2, and HO_2 in a gas discharge have been measured (*CJ3*).

(CK) On-Line Analysis. Ponchon has reviewed use of IR instruments as on-stream analyzers (*B29*) and Wilks has reviewed IR determination of composition of liquid streams (*B32*).

A new process IR analyzer uses reflection MIR to continuously monitor CO_2 levels in high gravity brewing and packaging operations (*CK1*). IR absorption has been used for on-line determination of moisture for control of the phosphate drying process (*CK2*). Differences between IR process analyzers and laboratory IR spectrometers have been discussed (*CK3*) (*CK4*). An on-line liquid stream analyzer using a multiple internal reflection flow through cell has been described (*CK5*).

(D) BIOLOGICAL-PHARMACEUTICAL APPLICATIONS

Various reviews have appeared on use of IR in the Biological–Pharmaceutical area, mainly on conformations of proteins (*B10*), (*B24*), (*B25*), (*B64*), (*B67*), (*B96*), (*B135*), (*B144*).

A collaborative study by 13 labs on problems connected with use of IR reference spectra for regulatory purposes has been reported. Spectra of 5 pairs of closely related compounds were used for reference. Differentiation between pairs of closely related compounds was successful. It was concluded that in *regulatory* tests both the *presence* of similarities and the *absence* of dissimilarities should be confirmed (*D1*). IR spectra have been used for identification of several antidepressant and hypnotic drugs and tranquilizers in unknown tablets and urine of patients (*D2*). Temperature dependence of the kinetics of disappearance of the 1952 cm^{-1} band of heme–CO in the dark and replacement by an intense band of Cu–CO at 2062 cm^{-1} in strong visible light has been followed by FT–IR (*D3*). An IR method has been described for determining lecethin and sphingomyelin in ~2 hours (*D4*). An IR method has been described for determination of staphylomycin (*D5*). IR spectra of globular proteins, Hb, bovine serum albumin, RNase, β-lactoglobulin, and α-casein in water have been compared with spectra of cast films (*D6*).

(DA) Urinary Calculi. The first Nordic quality control program on urinary calculi included 9 specimens and 9 components and 57 labs. Of the participating labs, 67% used a binary scale (Qual) and 80% were unable to carry out the analyses on 10 mg. or less. No difference between the reliability of IR spectrometry and wet chemical methods was observed (*DA2*). In a comparison with qualitative wet chemistry, IR analysis of urinary calculi showed greater reproducibility, more uniform sensitivity, and required smaller samples (1 mg.) (*DA3*), (*DA1*).

(DB) Blood Compatibility of Polymers. A FT–IR technique using attenuated total reflectance has been developed for studying protein adsorption from blood on surfaces. High quality spectra of protein adsorption are taken at 5 second intervals ex-vivo with a beagle dog as source of whole, flowing blood (*DB1*). FT–IR has been used to study adsorbed layers of blood proteins on polymer surfaces and to monitor formation of these layers directly from aqueous solutions (*DB2*).

(DC) Biological Monitoring. A spectrophotometer designed to measure simultaneously traces of deuterium oxide (12mg/L) and indocyanine green (0.12mg/L) in flowing blood has been described (*DC1*). Laser absorption spectroscopy by attenuated total reflection has been reported for in-vivo, non-invasive determination of glucose, polypeptides, urea, and cholesterol in blood (*DC2*). IR determination of ^2H_2O in biological fluids has been discussed. Arterial and urinary disappearance curves of ^2H_2O, measured over several days, permit calculation of total body water, daily water turn-over, and the half-time of water in the body (*DC3*). An IR method for determining CO in blood in the range of 1–10 ml CO/L has been described. Blood gases were trapped and measured

by IR after adding H_3PO_4 to 1 ml of blood after treatment with antifoam silicone Rhodorsil 426R (*DC4*).

(DD) Biological Membranes. Infrared membrane spectroscopy has been reviewed by Fringeli and Guenthard (*B54*). A Perkin-Elmer IR data station has been used to determine difference spectra of lipid–water systems, reconstituted lipid–protein systems, and a natural biomembrane (*DD1*). FT-IR is an extremely sensitive means for monitoring changes in both model and natural membranes induced by external factors such as temperature or external perturbants (*DD2*). FT-IR and far-UV CD both indicate that the visual transducing membrane protein, rhodopsin, contains extensive α-helical structure which is oriented predominantly perpendicular to the membrane plane (*DD3*). FT-IR has been applied to the intact and deproteinated plasma membranes of Acholeplasma laidlawii enriched biosynthetically with perdeuteriopalmitoyl chains. Temperature dependent behavior was monitored via the CD stretching modes and compared with that for the model membrane 1,2-diperdeuteriopalmitoyl-*sn*-glycero 3-phosphocholine (*DD4*). In the IR spectra of rib cartilage preparations, intensity of absorption peaks at 1030–1080 cm^{-1} have been reported to increase with age, whereas that for the 1240 cm^{-1} peak decreases with age (*DD5*).

(E) ENVIRONMENTAL APPLICATIONS

NO has been determined in cigarette smoke by non-dispersive IR (NDIR) (*E1*). A new technique which makes use of permeation through a silicone membrane in combination with an IR gas analyzer has been described for measuring CO_2 concentrations in stored goods, air layers in plants, and other sources (*E2*).

(EA) Contaminants in Water. An IR method for continuous monitoring low ppm levels of water in chlorinated organics has been reported (*EA1*). Sampling of petroleum containing wastewaters and their analysis by IR and other methods has been described (*EA2*). Gas chromatography combined with on-line FT-IR has been used for determination of α-chloroacetanilides in water (*EA3*).

(EB) Dust. Direct on-filter IR, redeposited IR, and x-ray diffraction have been compared for determining free crystalline silica (*EB1*). A study has been reported which concludes that effective determination of both amorphous and crystalline SiO_2 can be achieved with a combination of IR and x-ray diffraction (*EB3*). An analytical technique based on sensitivity, stability, and computerized data handling capability of FT-IR has been developed for identifying individual inorganic species in complex particulate pollutant mixtures (*EB4*). An IR method using ATR has been described for determining respirable quartz down to ~10μg (*EB5*). Qualitative IR analysis of tarry material deposited in some Egyptian cities showed the major constituents to be alkanes, phosphines, and Si–H containing compounds (*EB6*). Organic materials on airborne dust have been determined by IR after solvent extraction (*EB2*).

(EC) Atmospheric Monitoring. Continuous IR recording has been compared with a passive personal sampler for determining exposure to DMF in workroom air (*EC1*). IR monitoring of flue gases from a refuse incinerator containing HCl and SO_2 >160° in the presence of water vapor has been discussed (*EC2*). Advantages and disadvantages of IR analysis, including multi-station IR ambient air monitors, for toxic vapor analysis have been discussed (*EC3*). Continuous HCl measurement in flue gas from waste incineration by IR absorption using the Spectran 677IR has been reported (*EC4*). $Ni(CO)_4$ at sub-ppb levels has been successfully monitored in a plant environment by FT-IR and plasma chromatography with good side-by-side correlation (*EC5*). Absorption bands of α- and β-pinenes in the 8–14 μm atmospheric window have been reported to be intense enough for detection of naturally occuring terpenes at the 100 ppb level at 1 km. path length (*EC6*).

(ED) Stratosphere. An experimental approach for inverting IR heterodyne measurements of stratospheric trace constituents has been described for retrieving concentration profiles (*ED1*). FT-IR minimum detectable quantities have been determined for 14 trace atmospheric gases. Airborne detection of gas in an exhaust plume from an aircraft engine or in a waste gas plume from a stationary source has been described (*ED2*). The temperature profile of a methane/coal burner has been measured by taking the ratio of a pair of CO vibration–rotation lines with a tunable diode laser system (*ED3*). Altitude profiles of NO and NO_2 have been measured during a flight of a balloon-borne pressure-modulator radiometer (*ED4*). Remote IR spectrometry with 0.015–0.020 cm^{-1} resolution has been used to obtain profiles of HCl and HCHO concentrations in the atmosphere to ~45 km (*ED5*). The Limb Radiance Inversion Radiometer (LRIR) experiment on the Nimbus 6 spacecraft for determining ozone distribution in the atmosphere has been described (*ED6*). Peaks from NO_2, OH, HCl, and CO in far IR emission spectra of the stratosphere have been obtained by a rapid-scanning Michelson interferometer at resolution of 0.08 and 0.04 cm^{-1} (*ED7*).

(F) POLYMER APPLICATIONS

Several reviews of applications to polymers have appeared (*B23*), (*B44*), (*B53*), (*B69*), (*B77*), (*B81*), (*B82*), (*B96*), (*B114*), (*B115*), (*B141*). An IR spectrometric method for determining residual catalyst down to 100 ppm in commercial polyethylene has been reported (*F1*). IR spectroscopic studies of amorphous poly(ethylene terephthalate) annealed at 50° to and beyond embrittlement showed that the gauche conformation of $-OCH_2CH_2O-$ increases, and that other changes occur corresponding to embrittlement (*F2*). FT-IR was used to study variation of crystallinity of both components of blends of bisphenol A polycarbonate and polycaprolactone (*F3*). Bonding information for surface and bulk of ethylenediamine–methylenedi-p-phenylene isocyanate–polypropylene glycol copolymer has been obtained by FT-IR. Bulk and surface structures were quite different (*F4*).

Reflection–absorption IR spectrometry has been used to determine the structure of films formed by adsorption of $NH_2(CH_2)_3Si(OEt)_3$ onto Fe mirrors from aqueous solution (*F5*). IR and Raman spectra have been reported for polyelectrolytes formed between polyethylene oxide and NaBr, NaI, NaSCN, $NaBF_4$, $NaCF_3SO_3$, KSCN, RbSCN, and CsSCN (*F6*). Structure of frictional polymers formed on mated Pd/Pd pairs exposed to air–hydrocarbon vapor involving C_6H_6 has been studied by FT-IR (*F7*). Computerized IR has been used to characterize glass-reinforced Epon 828 crosslinked with methyl nadic anhydride via factor analysis and least squares fitting of spectra (*F8*) (*F14*).

FT-IR spectra have been used to analyze microtomed S-cured, carbon-black reinforced SBR samples (*F9*). FT-IR absorbance difference spectra have been used to study the mechanism of tertiary amine-catalyzed epoxide polymerization (*F10*). Problems associated with sample preparation, spectral data analysis, refraction and reflection at poly(ethylene terephthalate) fiber surfaces have been discussed relative to FT-IR analysis (*F11*). Surface brominated single crystals of hydrogenated polyethylene have been studied by IR (*F12*).

The trans–gauche concentration in crystalline polyethylene has been determined from the ratio of the CD_2 bands at 646–51 cm^{-1} for trans–gauche bond pairs and 620 cm^{-1} for trans–trans bond pairs (*F13*). Presence of methylolmelamine resin and polyethylene softener on shrink resistant wool have been detected by IR after chemical or solvent preconcentration (*F15*). C–H stretching and bending vibrations of methylene, α-methyl, and ester methyl groups of poly(methyl methacrylate) have been assigned on the basis of spectra of selectively deuterated polymers (*F16*). An analytical method for obtaining FT-IR spectra corresponding to the 1st and 2nd layers of laminated polymers via ATR has been described (*F17*).

Reactions responsible for formation of internal stresses during heating of acrylic fibers in air have been identified by IR spectra and kinetics of internal stress formation (*F19*). Positions and dichroisms of the major far infrared absorption bands of Kevlar fibers and fabric have been reported (*F20*). An IR study employing computer-assisted subtraction indicates that the gel form of isotactic polystyrene is in a different conformation from the usual 3_1 helical crystal structure found in amorphous and crystalline polymers (*F18*).

Raman spectra of α-D-glucose, β-D-maltose, D-cellobiose, and dextran in H_2O and D_2O and IR spectra of D-glucose-6,6-d_2, -1-d_1, and -1,2-d_2 have been reported together with assignments for COH, CH_2 and CH vibrations (*F21*). Volume fractions of trans and gauche glycol conformations of poly-

(ethylene terephthalate) were determined as a function of annealing by FT-IR (*F22*). The degree of branching of commercial samples of polyethylene crystallized from the melt has been determined by IR spectrometry using computer decomposition of bands in the 1320–1400 cm^{-1} region (*F23*).

(FA) Effects of Water in Polymers. FT-IR has been used to characterize interaction of nadic anhydride–crosslinked Epon 828 film with sorbed H_2O vapor (*FA1*). Apparatus has been described for measuring sorption–desorption by IR in transparent polymer films at a controlled strain or stress (*FA2*). The decrease of absorbance of OH^- and NH^- absorption bands during diffusion of D_2O vapor has been used to evaluate permeability of polyurethane films to H_2O vapor (*FA3*).

IR spectra of deuterated nylon 6 before and after rehydration showed well resolved ND bands which were resistant to rehydration (*FA4*). Cure characteristics and moisture uptake of 1009 epoxy resin have been studied by FT-IR (*FA5*). FT-IR has been used to monitor effects of counterion type and degree of hydration on anionic sites of a perfluorosulfonate ion exchange resin (Nafion) (*FA6*).

(FB) Plasma Treated or Produced Polymers. FT-IR has been used to analyze the surface of low density polyethylene which had been fluorinated to a depth of ~40–50A in a cold plasma in a 5% mixture of F in He (*FB1*). Polymer films prepared from CH_4 and Me_4Si or Me_4Sn have been studied by IR absorption before and after exposure to air (*FB2*). IR spectra of glow discharge polymerized poly(vinylidine fluoride) showed only broad absorption bands while commercial films showed sharp bands (*FB3*).

Thirteen nitrogen containing compounds with different unsaturation numbers have been polymerized in glow discharges, and formation of cyano and analogous groups investigated by IR (*FB4*). Plasma-treated poly(p-xylylene) and chlorinated poly(p-xylylene) have been studied by transmission and internal reflection IR. Transmission spectra showed no carbonyl band, but internal reflection spectra showed carbonyl bands at 1730 and 1640 cm^{-1} (*FB5*). FT-IR internal reflection spectra have been used to determine optimum glow discharge parameters for surface modification of low density polyethylene (*FB6*).

(FC) Orientational Measurements. Measurements on copolymers of C_2H_4 with various low moleculer weight olefins show that the dichroic ratio of the methyl group absorption of stretched films can be used to determine short chain branching. This type of branching is not easy to determine by IR absorption alone (*FC1*). To determine orientation of α-helices of proteins in photosynthetic membranes, polarized IR has been used to measure dichroism of the amide I and II absorption bands of air-dried oriented samples of purple membranes, chloroplasts, and chromatophores (*FC2*). Experimental possibilities of FT-IR for studies of crystallization, orientation, and relaxation in polyethylene film have been discussed, as well as experimental results relating to changes during stretching and relaxation (*FC3*).

FT-IR transmission and internal reflection spectra have been used to characterize polyethylene and polypropylene surfaces and to compare their degree of crystallinity and molecular orientation with bulk properties. To improve the accuracy of surface orientation measurements, a rotatable sample holder which is described in Section (*HF*) has been developed (*FC4*) (*HF2*). IR spectra of uniaxially drawn poly(ethylene terephthalate) have been determined as a function of applied strain. Using various computational techniques, observed changes in IR spectra have been related to the relaxed stress–strain curve of the film (*FC5*).

Intensities of six orientations of the polarization vector for the 1017 and 875 cm^{-1} bands relative to the direction of drawing have been measured for poly(ethylene terephthalate). With Raman intensities of the 1515 cm^{-1} band for 36 combinations of the electric vector of incident and scattered radiation, this has permitted evaluation of 7 orientation distribution parameters (*FC6*). Directions of transition moments for carbazole, 3-indoleacetic acid, 3-indolepropionic acid, 3-indolebutyric acid, and terephthalonitrile in drawn polyethylene films have been determined from IR dichroism of NH and CN bands (*FC7*).

(FD) Stress Effects in Polymers. Effect of temperature on vibrational frequency shifts in mechanically stressed polymer chains has been analyzed in terms of a temperature dependent frequency shift coefficient α_c. The predicted linear dependence of α_c on temperature is in qualitative agreement with experimental studies of stress-induced IR frequency shifts vs. T in isotactic polypropylene (*FD1*).

A difference spectrum method has been used to measure vibrational frequency shifts in uniaxially stressed ultraoriented isotactic polypropylene (*FD2*). Molecular level changes due to external stress have been studied in polystyrene film by a dynamic IR spectroscopic technique using FT-IR (*FD3*). IR spectra show that local structure is developed in electrically polarized polyacrylonitrile via appearance of fine structure in the nitrile absorption band (*FD4*). Deformation of oriented viscoelastic isotactic polypropylene has been examined in terms of time-dependent molecular stress distributions, orientation changes, conformation variations, and chain fracture (*FD5*).

(FE) Polymer Degradation. Kiran and Gillham have reviewed pyrolysis–molecular weight chromatography–vapor phase IR for analysis of polymers (*B35*). Time dependent data on selective oxidation of polyethylene with nitric acid show bands at 1710 ($-CO_2H$), 1650 ($-ONO_2$), and 1550 cm^{-1} ($-NO_2$) (*FE8*). Kinetics of thermal degradation of acrylonitrile–vinyl acetate copolymer, acrylonitrile–methacrylic acid copolymer, acrylamide–acrylonitrile copolymer, and PAN have been determined by FT-IR (*FE7*). Inhibited autoxidation of *cis*-1,4-polybutadiene rubber in the presence of 2,6-di-tert-butyl-4-methylphenol, 4,4'-methylenebis-(2,6-di-tert-butylphenol), and N-phenyl-2-naphthylamine has been studied by FT-IR (*FE6*). Reflection and transmission IR has been used to detect presence of overstressed bonds produced on surfaces by quenching and in the bulk by applying a load (*FE5*).

The effect of stress on the ozonolysis rate of isotactic polypropylene has been studied by attenuated total reflection (*FE2*). Three cured epoxy resins have been studied under various degradation conditions by FT-IR (*FE1*). Hydrolysis of solid bisphenol A polycarbonate, unstabilized to hydrolysis, has been studied by IR and UV (*FE4*). IR has been used to study oxidation of blends of polystyrene and poly(2,6-dimethyl-1,4-phenylene oxide) over the entire compositional range by singlet O from a microwave discharge, dye sensitized and photochemical oxidation (*FE3*).

(FF) End Group Analysis. The possibility of OH end groups in polyethylene has been investigated by IR spectra of OH and C–O stretching vibrations in olefinic molecular chains. Results were negative (*FF1*). Determination of molecular weights of polyethylene glycol by IR has been compared with other methods (*FF2*). The number average molecular weight of silane-terminated dimethylsiloxanes has been determined by comparison of the slope of absorption vs. concentration for the polymer with that for 1,1,3,3-tetramethyldisiloxane (*FF3*).

(G) INFRARED INSTRUMENTATION

Both Bode (*B18*) and Elliot (*B38*) have reviewed infrared detectors. The status of transmittance standards for infrared spectrometers has been reviewed by Lukasiewicz-Ziarkowska (*B27*) and wavenumber standards by Cole (*B106*). Use of a synchrotron for far infrared spectroscopy has been reviewed by Yarwood (*B33*). Background noise of a Ge–Cu photoconductive detector was reduced by using a grating cooled to 90 K. NEP at 12μ was 2×10^{-12} W. Spectra of heavily doped polymers with average transmittance of 10^{-3}% have been measured with this apparatus (*G9*). The ANDROS prototype hand-held IR absorption detector is sensitive to concentrations of CH_4 <5% which is claimed to be beyond the range of catalytic combustion sensors (*G1*). A photometric integrating sphere for both relative and absolute measurements of reflection coefficients of materials with arbitrary scattering indices in the IR has been described (*G2*).

Preparation and basic properties of glass materials for production of waveguide filaments transmitting energy in the far IR region have been described (*G3*). $ZnCl_2$ optical fibers have been fabricated with extremely low loss characteristics in the IR portion of the spectrum (*G10*).

Conclusions concerning the ultimate properties of long wavelength order sorting filters have been reported (*G4*). A new nondispersive IR (NDIR) modulation technique which is claimed to dramatically improve analytical sensitivity and zero stability has been described (*G5*). The technique of

Zeeman modulation spectroscopy has been applied to the NO fundamental in order to compare observed line shapes and intensities with theory (*G6*). A fast response dispersive IR analyzer has been described for simultaneous on-line determination of nitrous oxide and either halothane or enflurane (*G8*). A method is described for specific detection and quantitative determination of organic compounds containing oxygen in mixtures separated by gas chromatography. Oxygen is converted to CO with carbon at 1120° and detected by IR (*G7*).

(GA) Cells and Sampling Accessories. A stainless steel cell with AgCl windows for IR studies of low level impurities in corrosive liquids, such as Si and Ge halides, has been described (*GA1*). A high-temperature flow reactor for kinetic and spectroscopic studies at 300–1500K has been described (*GA2*). Spectroscopic flow reactors have been developed for the study of solid–fluid interactions by IR spectroscopy up to 450° C. and 60 MPa (*GA4*). Apparatus has been developed for study of adsorption on single crystal surfaces by reflection–absorption IR spectroscopy, LEED, and other techniques (*GA5*). A device for supporting up to 12 microgram samples for infrared analysis has been described (*GA6*).

A 1 meter long multipass cell for absorption measurements with laser radiation has been described which provides effective path lengths between 3 and 150 meters (*GA7*). A simple IR spectroscopic flow reactor has been described and examples given of its use (*GA8*). A multiple sample cryostat for far-IR transmission and photoconductivity studies at temperatures of 5–300 K has been described (*GA9*). A single pass heated metallic gas cell for corrosive materials which can be introduced in the solid, liquid, or gas phase has been described (*GA10*). A high pressure cell for far-IR absorption has been designed with dimensions small enough to be attached to the cold finger of a cryostat (*GA11*). A vacuum lock has been reported for introducing samples into a vacuum spectrometer without breaking vacuum (*GA12*).

A microreactor has been developed for studying heterogeneously catalyzed gas phase reactions in the 100–600 ° range by IR emission for use with a Fourier transform IR spectrometer (*GA13*). A Pfund-type absorption cell for gas spectra up to 1300K is described and contrasted to the White cell for high temperature measurements. (A Pfund-type cell is an axial arrangement with two pierced spherical mirrors) (*GA14*). A cell for investigation of gases over a wide IR range at pressures from a few torr. to 300 bar has been described (*GA15*). Simultaneous measurements of mass changes and spectra have been accomplished by suspending the substrate from one arm of an automatic recording microbalance in a vertical plane with the infrared beam incident in a horizontal plane (*GA16*).

A flow-through, hermetic, heatable cell for IR studies of surface compounds has been described (*GA17*). An improved technique for coating FT-IR light pipes with gold via mechanical firing has been described (*GA18*). Modification of the CIRA 101 chromatographic IR analyzer for introduction of liquid or solid samples has been described (*GA19*). An IR cell has been described which acts as a differential plug-flow reactor for spectra and catalytic activities simultaneously under controlled reaction conditions, with provision for in situ preparation of catalyst wafers (*GA20*).

(GB) Spectrometers. A computerized IR microspectrophotometer designed to determine the thickness of submerged films such as buried SiO_2 or Si_3N_4 in ion-implanted semiconductors, or photoresists has been described (*GB1*). A double-beam spectrophotometer with a multipass absorption cell has been developed to determine CO, CO_2, NO_2, SO_2, CH_4, and H_2S in the atmosphere. A 0.1–0.2 cm^{-1} resolution, ~1% accuracy, and a 100-m effective pathlength were required to attain ~1 ppm detection limit (*GB2*). A description of the computation system for a high resolution far IR Fourier spectrometer has been reported. Methods used for correcting erroneous sampling and for digital filtering are described (*GB3*). The efficiency of an emissionless IR diffuse reflectance spectrometer (EDR) is reported to be ~3 times that of a conventional diffuse reflectance spectrometer (DR) (*GB4*). A method of reconstructing the IR spectrum from the interferogram of the Fabry-Perot interferometer has been described for cases where the reflectivity depends on wavelength (*GB5*). Design and construction of an IR spectrophotometer for the quantitative measurement of attenuated total reflection spectra has been described. The instrument has been used to determine optical constants of liquids (*GB6*).

A middle resolution spectrometer with a symmetrical z-shaped setup in a vertical plane has been described. The arrangement with the slits over and under the grating reduces coma and eliminates unwanted reflections (*GB7*). Application of the Model 580 spectrometer with computer to spectra of CO, benzene vapor, carbonyl compounds, and biochemical samples has been described (*GB8*). A balloon-borne far-IR spectrometer for the investigation of extended sources incorporates a new technique for large angle surveying of IR emission from the Galactic Disk (*GB9*). A 3-m vacuum grating IR spectrometer with digital recording has been described. Resolution is better than 0.025 cm^{-1} at 3000 cm^{-1}, and details are given of a fast deconvolution procedure by which resolution is enhanced to near 0.010 cm^{-1} (*GB10*). A computer-spectrometer system for IR spectra has been described which has the novel feature that the computer modifies the scanning characteristics as the data are being acquired (*GB11*). A new interference spectrometer for the far-IR using the method of "selective modulation" has been described (*GB12*).

(GC) FT-IR. Various topics related to FT-IR have been reviewed (*B70*), (*B71*), (*B72*), (*B78*), (*B85*), (*B86*). Apodization of the interferogram of a high resolution Fourier transform IR spectrum has been accomplished by a convolutional method (*GC1*). The 30–370 cm^{-1} spectral region is obtained with a single measurement by combining two interferometers with Mylar beam-splitters of different thickness (*GC2*). A systematic error arising from radiation from the detector port of an interferometer is particularly significant at long wavelengths and when the specimen temperature differs from that of the interferometer (*GC5*). A study of effects of apodization on bandshape and resolution has been presented with particular attention on intensity considerations in the computed Fourier transform IR spectrum (*GC6*).

A new method for cancellation of systematic effects in comparison of different spectra recorded with a general purpose high resolution Fourier spectrometer is claimed to improve sensitivity and precision by two orders of magnitude (*GC3*). Fourier transform IR spectrometers designed around polarizing Michelson interferometers (PMI) have been predicted to cover much wider spectral range due to the achromatic nature of metal grid polarizing beam splitters (*GC4*). A dual-beam Fourier transform IR spectrometer for study of adhesives on metal surfaces switches the beam from the substrate mirror to a clean reference mirror without breaking the purge (*GC7*).

A Grubb-Parsons cube interferometer has been adapted for use with a high-pressure diamond cell with 2.5mm dia. windows (*GC8*). A refractive scanning system for interferometers has been described which reduces the alignment requirement for the scanning mechanism and the criticality of position measurement significantly relative to requirements for moving mirror interferometers (*GC9*). Superiority of a double-beam, optically compensated, Fourier transform spectrometer for measuring weak spectral features has been demonstrated, and the phase correction procedure for the compensating mode has been discussed (*GC10*). Design, calibration, and performance of the Voyager Michelson interferometer with its 50-cm diameter primary mirror and .25° field of view have been discussed along with a sample spectrum of Jupiter (*GC12*).

A vacuum IR interferometer for use to 5 cm^{-1} has been described with examples from vibrational spectra of gases (*GC13*). Improved sensitivity has been reported for dual-beam Fourier transform IR spectroscopy by using a new Digilab 496 interferometer (*GC14*). FT-IR has been applied to studies of the solid/gas interface where it permitted solid and gas phase contributions to be filtered out to produce detailed spectra of the monomolecular interface (*GC15*).

(GD) Laser Spectrometers. Several reviews have appeared on infrared lasers (*B15*), (*B20*), (*B40*), (*B60*), (*B105*), (*B107*), (*B118*). A versatile IR laser system capable of generating picosecond pulses continuously tunable from 3.3 to 8.4 μm, with peak powers of 1–20 MW has been described (*GD1*). A coherent spectrophotometer tunable from 1.45 to 20 μm has been described. The source is a $LiNbO_3$ optical parametric oscillator pumped by a Nd-YAG laser, and Ag$GaSe_2$, GaSe, or CdSe crystals are used as down converters

(*GD2*). A high resolution IR spectrometer for the 2.2 to 3.3 μm range has been developed using a computer controlled continuous wave color center laser. Computer control permits single frequency scans of up to 100 cm^{-1} (*GD3*). A method of direct frequency reading IR spectroscopy that uses tunable electrooptically generated CO_2 laser sidebands has been described (*GD4*).

Tunable diode lasers (TDL's) offer the potential of fine grain spectroscopic measurements in the 0.3–34 μ spectral region (*GD5*). A diode laser based IR heterodyne spectrometer for lab and field use has been developed for high efficiency between 7.5 and 8.5 μ (*GD6*). Results have been reported using a powerful, narrow band, continuously tunable dye laser with different Raman media to create tunable wavelengths from near IR up to submillimeter waves (*GD7*). A 2nd derivative technique has been developed by which accurate IR line widths and shapes may be measured using a single beam tunable diode laser spectrometer even in the presence of a sloping background (*GD9*).

A detailed experimental system analysis has been reported for the upconversion of CO_2 laser radiation into the working range of photomultipliers using the ternary semiconductor $AgGaSe_2$ as the nonlinear crystal (*GD10*). The application of a high liquid pressure chamber with a liquid pressure transmitting medium to diode laser tuning has been reported to be useful for high resolution spectroscopy (*GD8*).

(H) TECHNIQUES

An experimental FT–IR method for determination of the complex *n* of a very heavily absorbing liquid at submillimeter wavelengths has been described (*H1*). CO and temperature measuring methods have been reported for the post–flame region of laminar, premixed CH_4/air flat flames by laser absorption spectroscopy and conventional probe techniques using nondispersive IR analyzers for CO and CO_2 (*H2*). The method of E. Korte (1978) has been modified to measure the IR rotatory dispersion (IRD) of induced cholesteric phases with a minicomputer coupled Fourier spectrometer (*H3*).

Small transmission losses of NaCl, KBr, TiCl, KRS–5, CsI, and PbI_2 near 10 μm have been measured using an improved differential IR spectrometer with an accuracy of >0.1% in transmittance (*H5*). Operation and performance characteristics of nondispersive IR gas analyzers for determining H_2O vapor continuously in a wide temperature range have been described (*H6*).

Fermi resonances in the IR spectra of $CaSO_4$–doped KI and KBr have been studied by scanning pressure and temperature (*H7*).

(HA) Sample Preparation. Linear dichroism of pyrene oriented by stretching in polyethylene has been studied using FT–IR spectroscopy and symetries of ~60 vibrations assigned and orientation factors determined unambiguously (*HA1*). A simple reflection method for measuring IR spectra of clay minerals utilizes Au coated glass slides on which the sample suspension is poured and dried (*HA2*). A simple technique for preparing mulls of compounds which are deuterated at active H sites has been described. A solution of the compound in an exchange solvent is mixed with nujol and the solvent is removed by evacuation (*HA3*). Thin–layer chromatography (TLC) combined with IR spectroscopy and the Wick–Stick method of Garner and Packer (1967) has been used for separation and identification of substances with low solubility (*HA4*).

The IR spectrum of 1/4 in. wide Teflon tape permits its use as an IR window material, for example, with a sample sandwiched between 2 layers (*HA5*). The combination of microscale HPLC and IR spectrometry with a KBr disk buffer memory for collecting fractions prior to spectral measurements has been described (*HA6*). Preparation of monofilaments for IR spectroscopy using a support matrix with a lower m.p. and a refractive index similar to the polymer film has been described using poly(p–benzamide) and polyethylene as monofilaments and support matrix, respectively (*HA7*). A micro pyrolysis method for identification of <1 mg. of vulcanazates and filled plastics has been described (*HA8*). Use of the diamond anvil cell with a 4X beam condenser in IR analysis in the fields of forensic science, industrial coatings, drugs and pharmaceuticals, polymers, inorganics, minerals, coal, and pollution has been demonstrated (*HA9*).

(HB) Time Studies. The extraordinary attention to detail which is required to make meaningful time–resolved FT–IR measurements for repetitive events with time constants shorter than the single scan time has been discussed (*HB20*).

Thermal decomposition of kraft lignin has been studied by FT–IR evolved–gas analysis, a technique designed for on–the–fly, simultaneous monitoring of multiple vapor–phase species (*HB5*) (*HB13*) (*HB22*). Use of FT–IR spectrometry for analyzing the gaseous decomposition products evolved during thermogravimetric analysis has been discussed and illustrated by industrial analytical examples (*HB8*). A continuous FT–IR monitor for the total gaseous effluent from a heterogeneously catalyzed chemical reaction has been described (*HB17*).

Mechanism of the carbon–steam reaction catalyzed by decomposition products of K_2CO_3 was investigated by temperature programmed desorption and in–situ FT–IR spectrometry (*HB3*). Kinetic and spectroscopic characterization by FT–IR has been reported for the gas–phase reaction between O_3 and C_2H_4 (*HB6*). FT–IR has been used to monitor the ~200K order–disorder phase transition of anthracene–cyanobenzene charge transfer complexes (*HB10*). FT–IR has been used to determine the lifetime of the active catalytic species in pentacarbonyliron(0) photocatalyzed olefin isomerization (*HB12*). A formal integration technique of analyzing absorbance–time data has been reported (*HB16*). The self–reaction of HO_2 has been studied by FT–IR in the photolysis of Cl_2 in the presence of H_2 and O_2 (*HB18*).

Tunable IR pulses between 2500 and 7000 cm^{-1} have been used to study dynamics of vibrational modes of polyatomic molecules. The first IR pulse excites a particular vibration. The second, monitors the instantaneous state of the vibrational system (*HB14*). Synchrotron radiation from storage rings provides time resolution in the picosecond range for spectroscopy from the IR to the x–ray region. Status of time–resolved experiments at storage rings has been discussed (*HB25*). A flash photolysis apparatus with monitoring IR beam allows measurements of relative transmission changes of 10^{-3} in a few milliseconds. It has been used to investigate photodissociation of CO–myoglobin (*HB19*).

A multipass White cell is mounted downstream of a high temperature flow tube to monitor IR spectra of flowing gas species. A key feature is that the gas is aerodynamically confined to eliminate recirculation in the cell (*HB26*). An IR stopped flow machine based on a Perkin–Elmer 237 spectrophotometer has been described (*HB27*).

The non–linear optics basis and application of time–resolved IR spectral photography (TRISP), a new technique of nanosecond time–resolved IR absorption spectrometry have been described (*HB2*) (*HB9*) (*HB24*).

Simultaneous FT–IR and mechanical measurements have been used to characterize deformation and relaxation phenomena in polymers (*HB1*). Uniaxial deformation and recovery of amorphous poly(butylene terephthalate) was investigated by simultaneous FTIR spectroscopy and stress–strain measurements (*HB4*). Photooxidation studies of MeH=NMe and for Cl–initiated oxidation of CH_4 in O_2–N_2 mixtures has been studied by FT–IR (*HB7*). FT–IR spectrometry has been described in relation to orientation, necking, dichroic ratio, axis rotation, the effect of strain rate, stress–strain curves, and the effect of polymer density (*HB11*). Spectral changes during a simultaneously recorded stress–strain diagram have been reported (*HB15*). IR spectra have been continuously recorded during stretching of isotactic polypropylene using a rapid scanning FT–IR spectrometer (*HB21*). Use of modern FT–IR equipment for studies of crystallization, orientation, and relaxation phenomena in polymers is described and illustrated with measurements on polyethylene (*HB23*).

(HC) Reflection. IR absorption of molecular monolayers has been reported to be enhanced by a factor of 20 by thin metal overlayers or underlayers with use of the attenuated total reflection technique. Total enhancement, including contributions from ATR geometry, is almost 10^4 (*HC5*).

For metal surface studies of adsorbates which participate in charge–transfer with the metal, interpretation of IR data must consider strong electron density oscillations between molecules and the surface regardless of orientation. Devlin and Consani have pointed out that totally symmetric adsorbate modes produce such oscillations which dominate the IR spectra of charge transfer systems (*HC1*). Large electric field

gradients which exist near a metal surface have been shown to cause quadrupole allowed vibrations to become IR allowed under some circumstances (*HC2*). Conversion of incident radiation to surface electromagnetic waves has been studied by adjusting two coupling prisms and varying the angle of incidence. The most effective angle of incidence was about 0.2° less than the critical angle (*HC3*). Broadband generation and spectroscopic detection of IR surface electromagnetic waves (SEW's) has been reported from 600 to 1800 cm^{-1}. Comparison of SEW with surface reflection spectroscopy (SRS) indicates that the integrated absorbance of an absorption line is an order of magnitude larger with SEW than with SRS (*HC4*).

An external reflection IR study of poly(acrylic acid) on optical quality Al_2O_3 showed that a major fraction of adsorbed molecules are bound to the surface by carboxylate ion with undissociated acid groups exposed at the ambient polymer interface. This method is shown to be useful in determining the nature of adsorbed polymer films (*HC6*).

(HD) Emission. Molt has demonstrated the sensitivity and accuracy of an IR grating spectrometer with high performance optics and electronic recording. Recording of emission spectra of good quality by an IR grating spectrometer for samples at elevated temperature has been described. For study of thin films on metals this method offers advantages over other methods (*HD2*). The emission spectrum for a monolayer quantity of *p*-nitrobenzoic acid on a thin oxide coated, evaporated Cu substrate at 300 K has been studied with a cryogenic interferometer with good S/N in the 1250–2000 cm^{-1} region (*HD1*). A polarization modulation technique has been applied to obtain IR emission spectra of thin poly(vinyl acetate) and Al_2O_3 films on metal mirrors at 160°. Emission spectra of the films as thin as a few nanometers could be detected (*HD3*). The major limitations in FT-IR emission spectroscopy have been discussed and problems associated with multiple passing of radiation through the modulator are outlined. Sensitivity of the technique is illustrated with spectra of microgram quantities. Conditions which cause instrumental background and the method for removal are discussed. Background problems were more severe with cooled MCT detectors than with room temperature TGS detectors (*HD4*).

(HE) Diffuse Reflection. The quantitative relationship between diffuse reflectance intensity and concentration has been studied experimentally over the whole concentration range (*HE5*). Fuller and Griffiths report that diffuse reflectance techniques enable increased sensitivity for IR microsampling compared with KBr micropellets. Detection limits of <10 ng. of samples have been observed. Extraction of sample spots from TLC plates followed by deposition onto KCl yields better results than in-situ measurement of diffuse reflectance from the TLC plate (*HE1*). Instrumentation and applications of diffuse reflectance IR spectrometry for analysis of pharmaceutical tablets, coals, and minerals have been discussed (*HE4*).

Diffuse reflectance has been used to examine the effect of each step in the preparation of gas chromatograph packing materials coated with an ultrathin film of Carbowax 20M (*HE2*). A diffuse reflection device for a FT-IR spectrometer has been reported which transmits ~10% with a standard sample. Stray light measured without a sample was <1% of output of standard sample (*HE3*).

(HF) Attenuated Total Reflection. Internal reflection spectroscopy has been reviewed by Wilks (*B13*) and Zolorarev, Lygin, and Tarasevich (*B140*). For a sensitive measurement of surface molecular orientation by ATR IR dichroism, a sample holder has been developed for a thin square rhomb ATR plate which can be rotated without disassembling. This permits the orientation of the sample relative to the E-vector of incident radiation to be changed without changing the contact area (*HF2*). For depth profile measurements by ATR, either the incident angle of the ATR plate has been changed, or a thin spacer film, transparent to most of the IR radiation, was cast directly on the ATR plate. This reduced the depth of penetration of radiation into the sample to provide spectral information at various depths (*HF6*).

Attenuated total reflection IR spectra of uniaxially stretched *cis*-polybutadiene and polyisoprene vulcanizates indicates that surface orientation differs substantially from that within the sample (*HF1*). Advantages of recording ATR spectra with a FT-IR spectrometer have been pointed out for oil films in the range below 10 nm mean film thickness on Al foils (*HF3*). IR transmission and ATR spectra were measured for N-(p-ethoxybenzylidine)-p-cyanoaniline under the influence of an external d.c. electric field. The threshold voltage for reorientation was significantly different for surface and bulk (*HF4*). IR spectra of some model food materials have been recorded by ATR (*HF5*). Residues of 11 substituted ureas used as herbicides have been identified by IR microtechniques using ATR (*HF7*).

(HG) GC-IR. Griffiths has reviewed chromatography and FT-IR (*B73*). Combined data of GC/FT-IR and GC/MS have provided improved identification for a standard solution of priority pollutants. GC/FT-IR selectivity favors polar compounds and GC/MS favors nonpolar compounds (*HG1*). Initial results of joint use of IR and MS spectral information from a directly linked GC/FT-IR/MS combination has been shown to be effective in situations where MS or IR information alone would be inadequate (*HG8*). A comparison has been published between GC/FT-IR, HPLC/FT-IR, and GC/MS concerning the capability of each as a technique in the analysis of an industrial wastewater (*HG15*).

GC detection by matrix isolation Fourier transform IR spectrometry has been described. Eluates are deposited directly in the GC carrier gas on faces of a 12-sided movable Au-mirror mounted within the cold head of a closed-cycle cryostat (*HG2*). A new, selective IR dectector using a laser homodyne photothermal refractometer has been described. This technique, called Phase-Fluctuation Optical Heterodyne Spectroscopy (PFLOHS) has demonstrated sensitivity of 10^8/cm. This corresponds to <1 picogram of injected material in the case of SF_6 (*HG4*). A GC detector based on IR absorption of the CO_2 carrier gas has been described. Displacement of CO_2 by eluate is quantitated by IR determination of CO_2 passing through a permeable membrane, giving equal sensitivity for all eluates (*HG6*).

Detection limits of ~1 ng of injected sample have been demonstrated for Fourier transform IR of peaks eluting from SCOT columns using small, highly transmitting light-pipes in a dual-beam configuration (*HG11*).

An integrated gas chromatograph/Fourier transform IR system for analysis of environmental pollutants which employs many different techniques of sample introduction and manipulation has been described. Cold traps and collection cartridges permit recovery and additional fractionation of samples (*HG3*). Recent advances in gas chromatography/Fourier transform IR hardware and software for collection and analysis of GC/FTIR data have been described (*HG5*). Vapor phase IR spectrophotometry has been used on-line with stainless-steel porous-layer open tubular (PLOT) columns with Dexsil and other stationary phases for separating volatile metal chelates and organometallic compounds (*HG9*). Wide-bore WCOT columns have given improved separation as compared to support-coated open tubular (SCOT) columns for on-the-fly gas chromatograph/Fourier transform IR detection (*HG10*). GC-IR has been used to analyze semivolatile organic pollutants collected during coal gasification on a bench scale (*HG12*). A minicomputer controlled FT-IR spectrometric accessory to gas chromatographs has been illustrated by analysis of small samples (50 ng iso-Bu methacrylate), functional group analysis, and enhancement of unresolved chromatograms (*HG14*).

Gasoline fractions have been analyzed for alcohols, ketones, aromatic hydrocarbons and *tert-Bu Me ether* by a gas chromatograph with a MIRAN-1A® detector (variable wavelength filter and variable temperature flow through cell (*HG7*). Design, operation, and performance of a device for combining standard IR spectrometers with standard gas chromatographs using both in their normal manner has been described (*HG13*).

(HH) LC-IR. A liquid chromatograph with an IR spectrometer detector has been described for size exclusion chromatography of polyethylene and oligomers (*HH1*). Free fatty acids (as methyl esters) and mono-, di-, and triglycerides have been separated and quantitated by HPLC using an IR detector set at 5.72 μm (*HH2*). Pyrethroid insecticides in formulated material have been analyzed by HPLC using an IR detector at the carbonyl or the C-O absorption and a UV detector at 280 nm. The selectivity of the IR detector was such that aromatic solvents did not interfere. Minimum detectable levels for the IR detector were 1 μg for resmethrin

and permethrin and 2 μg for fenvalerate (*HH4*).

The high selectivity of a conventional IR spectrometer as detector for liquid chromatography has been demonstrated in the gel permeation chromatographic separation of a 7-component synthetic mixture of coal derived products (*HH6*). In the characterization of solvent-refined coal by size exclusion chromatography, the use of FT-IR detection allows simultaneous monitoring of multiple chemical functionalities (*HH3*).

A microcomputer interface between a high performance liquid chromatography and a diffuse-reflectance FT-IR (DRIFT) spectrometer has been described. The solvent is first concentrated by a factor of ~10 by a short heated tube and then passed dropwise into cups containing powdered KCl in a carousel. The DRIFT spectrum of each peak is measured after solvent elimination. Submicrogram detection limits are observed for all samples of low volatility and chromatographic resolution is maintained even for closely spaced peaks (*HH5*). A micro liquid chromatograph interfaced with a FT-IR spectrometer for on-line analysis of liquid chromatographic effluents has been described. About 2 μm of injected diethylphthalate can be detected using a 0.025 mm flowcell (*HH7*).

(HI) Photoacoustic Spectrometry (PAS). Photoacoustic infrared spectroscopy has been reviewed by Busse (*B46*), Patel (*B98*), and Kanstad and Nordal (*B102*). This technique is also called *optoacoustic* spectroscopy (OAS). The term *optoacoustic* has been in use for many years but the trend is toward use of *photoacoustic*. This is presently an area of rapid growth via photoacoustic detectors which can be attached as sampling accessories for FT-IR spectrometers.

The optoacoustic effect has been widely used in detectors for non-dispersive gas and vapor analyzers for many years (*5*), (*3*). Typically, the detector in such devices is sensitized by filling with gas containing the component to be detected. Radiation from a broad band infrared source is modulated at a frequency in the acoustic range (100-1000 Hertz). Pressure pulsations are produced in the detector chamber by absorption of the infrared beam. The pulsations are detected by a built-in sensitive microphone. This device is also known as a *spectrophone* (*3*). The usual arrangement in older devices is to place the sample cell between the infrared source and the detector. Thus, the selectivity of the detector is achieved by photoacoustic (or optoacoustic) means, but the device actually measures attenuation of the infrared beam as the difference between signals for the empty and filled absorption cell. This has been discussed in detail by Hill and Powell (*4*).

The present wave of photoacoustic detectors and spectrometers introduces the sample to be analyzed directly into the detector chamber either as a gas or as a condensed phase. Absorbed photons are detected by the effect they have on the sample and its surroundings, either via a gas thermometer (microphone) or piezoelectric or other detector. The photoacoustic spectrum looks like an emission spectrum. Background for a non-absorbing sample is nominally zero. This avoids many problems associated with with the usual measurement of absorption as the difference between incident and transmitted radiation.

There are presently two major ways in which the photoacoustic technique is being applied in infrared spectroscopy: (1) photoacoustic measurements over a narrow spectral range using fixed or tunable infrared lasers, and (2), photoacoustic spectra over a wide spectral range using either dispersive or FT-IR spectrometers for scanning.

The theory and applicability of photoacoustics has been discussed in detail in a new book by Rosencwaig (*A23*).

Photoacoustic measurements which make use of fixed or tunable lasers have the capability of high sensitivity due to the concentration of excitation energy in a narrow line. A number of molecular gases can be detected by photoacoustic methods at the CO_2 wavelengths between 9 and 11 μm (*HI16*). Vinyl chloride has been detected at <1 part in 10^8 in air using a photoacoustic system with a tunable CO_2 laser (*HI17*). Photoacoustic spectra of skin lipids have been measured using piezoelectric detection with a low-power CO_2 laser at 1/100 the concentration required for transmission spectroscopy (*HI10*). A small non-resonant cell, together with a low power semiconductor laser, have been used to measure CO at concentrations as low as 50 ppmv (*HI9*).

FT-IR spectrometers are well matched to the PAS detector. The interferometer modulates the radiation from the (globar) source in a broad band of acoustic frequencies which are linearly related to the infrared frequencies. Thus, in one instance, the 4000 cm^{-1} region is modulated at acoustic frequencies in the 1000 Hertz range, and the 400 cm^{-1} region, at acoustic frequencies in the 100 Hertz range. Several commercially available PAS detectors are designed to be set up in the sample compartment of a FT-IR spectrometer and plug-in directly in place of the usual TGS or MCT detector. Most of the work published in the last two years has been on PAS of solids, in which the thermal diffusion length and the optical penetration depth combine to give an effective PAS sampling depth. Increasing acoustic frequency reduces PAS sampling depth, so FT-IR/PAS sampling depth decreases at high optical frequencies. Thus, control of the mirror velocity affords a measure of control of sampling depth. The PAS technique works on irregularly shaped samples and powders. Since it is the *photons absorbed by the sample* which are detected, it is not necessary to collect radiation which is not absorbed and focus as much as possible on the detector as in the case of transmission spectra. Christiansen filter effects appear to be absent, and it is not necessary to mix the sample with KBr or other diluent to match refractive index. This reduces the chance of contamination. Clearly this is a very interesting and fruitful area.

The effects of Helmholtz resonance of the photoacoustic cell and of the thermal properties of samples in FT-IR photoacoustic spectroscopy have been discussed (*HI4*). The effect of particle size, and the question of whether PAS results are quantitative has been investigated with the result that the spectra of 0-5μ particles are stronger than for larger sizes (*HI5*). PAS provides a well resolved absorption band under circumstances where the Christiansen effect interferes with transmission measurements (*HI6*). Photoacoustic IR spectra in the 100-1500 cm^{-1} region for some ionic (LiF) and semiconducting (Ge, Si, GaAs) powders and crystals have been reported (*HI8*). Photoacoustic spectra of hemin, Hb, protoporphyrin IX, and horseradish peroxidase have been used to obtain structural information which cannot readily be obtained by normal transmission IR spectroscopy (*HI11*). Elimination of dispersion-induced distortion in infrared absorption spectra by FT-IR photoacoustic techniques has been demonstrated (*HI15*). Aging of coal surfaces, including both oxidation and abrasion, have been demonstrated in a comparison of photoacoustic IR spectra of freshly cleaved and aged coal surfaces (*HI18*). Versatility of FT-IR photoacoustic spectroscopy has been demonstrated by measuring a wide selection of IR spectra of opaque samples (*HI20*). Fourier transform IR spectroscopy of solids and liquids using photoacoustic detection has been reported and the advantages and disadvantages of photoacoustic spectra have been discussed (*HI22*).

The background for non-absorbing regions is theoretically zero, but most PAS spectra of solids show appreciable continuous background. There is also the problem of correcting the intensity of the PAS signal for the spectral variation of radiation which excites the PAS signal. The PAS spectrum of charcoal, which should absorb all radiation has been used to normalize the spectra. However, this procedure has been questioned by Low and Parodi (*HI14*), and Riseman and Eyring have concluded that *no* form of carbon is suitable for normalization of photoacoustic spectra (*HI7*).

PAS is not limited to Fourier spectrometers. Low and Parodi have described a dispersive photoacoustic spectrometer (*HI13*), and spectra of solids and surface species have been measured on such a spectrometer (*HI26*). Low and Parodi have also described a photoacoustic system coupled with a reactor in which samples may be treated with gases at 1000°.

Since PAS is a surface technique, one would like to use it to study surface reactions of powders which may not be readily prepared for transmission spectra. FT-IR/PAS has been used successfully for in-situ monitoring of reactions involving a gas phase species (*HI1*). Binding of vinyltrieth-oxysilane to hydroxyl groups on a silica surface has been identified by photoacoustic spectroscopy (*HI2*). In both cases residual gas pressure of reactants over the surface is small. When the surface is in equilibrium with vapor, it is necessary to deal with the fact that the photoacoustic detector is much more efficient for detecting photons absorbed by the vapor than for those absorbed by the surface of the solid. Thus, for example, it is necessary to take steps to reduce water vapor in the cell either by drying the sample, or as has been sug-

gested by Krishnan (*6*), by including a little drierite in the cell.

Until recently, it appeared that the integration times for photoacoustic spectra of solids were necessarily quite long. However, Krishnan has recently reported PAS spectra of solids with excellent S/N for integration times as short as 2 minutes (*6*).

(I) COMPUTER APPLICATIONS

Gram–Schmidt orthogonalization has been compared with low-resolution FFT integration for reconstructing gas chromatograms. FFT integration at 16 cm^{-1} yields more accurate relative peak heights and is adequate for on-line application. Gram–Schmidt orthogonalization when optimized can provide more sensitive total IR absorption detection than the FFT technique, but requires more computer time than transforming all spectra acquired (*I1*). An interactive minicomputer procedure for analysis of IR spectra based on full curve subtraction of spectra has been described (*I2*). Peri has reported that computerization of dispersive IR spectroscopy has greatly improved the sensitivity of this technique for studies of catalyst surface chemistry and has enabled the spectral data to be handled more quantitatively (*I3*). A technique for eliminating baseline variation by ultralow frequency filtering in the frequency domain (transform space) has been illustrated by applying it to diode laser spectra of ethane (*I4*).

The Perkin–Elmer IR data station, a computer system for processing, displaying, and identifying IR spectra, has been described (*I5*). Principles of two reduction methods, the group theoretical method and the isotopic reduction method, and their application to vibrational spectroscopic problems have been discussed (*I6*). A computer program has been described and illustrated for fitting dispersion formulas to IR reflection spectra. Highly correlated parameters, e.g. for overlapping reflection bands, are separated by Kramers–Kronig analysis (*I7*).

(IA) Computer Search. Craver, Kirby, and Jones have reviewed infrared spectral data coding (*B30*). A computerized search routine for identification of IR spectra using interferometric data exclusively has been described. Interferometric phase error and instrument function are removed prior to the search process (*IA1*). Library searching via Fourier transforms of IR spectra has been discussed. Searching in the time domain is more tolerant to noise than searches in the spectral domain, and fewer points are required to encode unique characteristics of spectra. Time-domain classification of IR spectra has been demonstrated, and the possibility of indexing the library for a binary search has been discussed (*IA2*).

Results of application of a computer search system based on the EPA library of digitized vapor phase IR spectra to a coal gasification sample have been described (*IA4*). A new computer program KISS for ASTM IR spectral data has been reported. KISS utilizes data on peak intensity of the sample spectrum as well as peak position (*IA3*). Evaluation of GC/FT-IR search system has been carried out via a series of experiments designed to examine differentiation among closely matching spectra, effects of spectral noise, effects of sloping baselines, and spectra from unresolved GC peaks. Excellent search results are obtainable when high-quality digital spectra are used as reference (*IA5*). An automated search and display system for matching IR spectra has been described which combines the use of the Sadtler Spec-Finder search database with an automated microfiche retrieval and display system for complete spectra (*IA6*).

A minicomputer-oriented chemical information system (KISIK) based on 3 different spectrometries (IR, MS, ^{13}C NMR) has been described. The system characteristics are substructure search, library searches on various files, and statistical handling of retrieved data (*IA7*). Forty three drugs have been identified by matching selected peaks of the fingerprint area of the IR spectra of known drugs using a Fortran program (*IA8*). Information theory has been used for objective evaluation of the efficiency of computer-aided spectra search systems. The influence of the following factors can be estimated: volume, structure, and quality of library spectra, efficiency of the encoding and comparing algorithms, and subjective errors involved in encoding of spectra (*IA9*). Four mathematical moments of an IR-spectrum as characteristic statistical parameters of the chemical compounds have been utilized for computer retrieval of IR spectra. The 1st (center of gravity), 2nd (standard deviation), 3rd (skewness), and 4th (kurtosis) moments were used (*IA10*).

(IB) Computer Data Bases. Current IR data collections and pattern matching methods for spectra identification in IR analysis have been discussed (*IB1*). The major changes in the current status of the Molecular and Crystal Data system which contains various spectroscopic data, structural, and physical properties of molecules and crystals has been described. The molecular vibration subsystem and the IR spectral data retrieval system are described (*IB2*). Research for the establishment of a spectral bank, not only for analytical use, but also for accumulation and storage of correct and reference spectral data, has been discussed for IR, Raman, NMR, ESR, and mass spectra (*IB3*). A data system has been described that allows storage of IR reference spectra, comparison with IR spectra of known substances, and rapid and certain identification of these substances. Examples show that the same reference spectrum is selected even when the spectrum of the unknown substance is considerably distorted (*IB4*). The computer search of IR spectra by the system SPEKSU has been reported. Significant information, adequate encoding, the significant spectral data for storage, and the criteria for two spectra to be considered identical or similar are examined (*IB5*).

(IC) Computer Interpretation. Schrader, Bougeard, and Niggemann have reviewed determination of organic structures by computer from vibrational spectra (*B31*). An automated IR interpreter, PAIRS, has been implemented on a Nicolet 1180 minicomputer. With a fast peak picking algorithm, the result is that one computer controls the entire IR experiment including acquisition, processing, and interpretation. Complete interpretation requires approximately the same amount of time as the original measurement. PAIRS determines functionalities as opposed to matching a spectrum to an individual compound (*IC1*). The diagnostic value of an interpretation system for vibration spectra has been investigated in relation to the number of structural units the system can cope with (*IC2*). The ASSIGNER analytical computer system determines the probability of existence of functional groups using on-line measured spectral data and off-line collected parameters. The system finds twice as many groups as are really present, but very seldom misses a functional group (*IC3*). Computer aided interpretation of ^{13}C-NMR and IR spectra of organic molecules is done by an artificial intelligence approach using ASSIGNER, a system for listing functional groups which are reasonable candidates for the final structural isomers. The procedure of finding possible functional groups and the main features of the filtering steps have been outlined (*IC5*).

The structure similarity and dissimilarity implied in many structure–property and structure–activity relationships has been examined from the graph theoretical point of view. The basis of the method is that all paths within molecular skeletons are enumerated and sequences of path numbers (i.e., the number of paths of different length) are compared (*IC4*).

Automatic interpretation of digital recorded IR and Raman spectra has been described. Spectra are reduced to band lists containing position, intensity, and half-widths of bands. The interpretation algorithm tests for presence or absence of characteristic bands or groups. A review of interpretation results shows that absence of structural elements is found more safely than presence (*IC6*). The CRISE computer program has been used to correlate wavenumber regions and six structural elements on the basis of two standard files of 579 IR and Raman spectra. The IR and Raman results for a structural element can differ appreciably, yet neither technique is clearly superior for interpretative purposes (*IC7*). The interpretative process for vibrational spectra has been considered in detail, including the concepts of the spectral data, the structural elements, and the basic data file (*IC8*). The procedure of transforming an IR transmittance spectrum into a mapping of a chemical compound has been analyzed (*IC9*). Determination of molecular structure using consecutive applications of experimental and theoretical spectroscopy, quantum mechanics, and computer analysis has been described. First, an automatic structure identification system, STREC, is applied to IR, Raman, UV, and mass spectra. The computer then constructs a spatial model and calculates vibrational and UV spectral curves for comparison with ex-

periment (*IC11*). A method has been described for direct analysis of interferometric data from GC/FT-IR experiments. A synthetic interferogram is initially produced which represents the characteristic absorption features of a particular functional group or compound class. A zero displacement correlation is performed between this test interferogram and each sample interferogram. Presence of the chosen functionality in the GC effluent is indicated by a small value of the resulting cumulative sum (*IC10*).

(ID) Factor Analysis and Multiple Regression. Target factor analysis (t.f.a.) criteria have been applied to FT-IR spectra in order to determine, without any prior knowledge of the experimental error, the number and identities of components in a series of related multicomponent mixtures. The t.f.a. method is also used for quantitative analysis and is compared to regression analysis, which force-fits the data and does not compensate for an impurity of small but measurable quantity (*ID1*). Application of FT-IR spectroscopy to the quantitative determination of mineral matter in coal by least squares curve-fitting has been described (*ID2*). Use of factor analysis, the absorbance ratio method, and least-squares curve fitting for evaluating FT-IR spectra of amorphous and semicrystalline poly(ethylene terephthalate), i.e., for determining chain conformations, has been discussed (*ID3*). Improved sensitivity and precision in determination of trace gases by applying new spectral least-squares methods have been reported. Relating all spectral information in the reference spectrum of a trace gas to that of the unknown sample and by appropriately fitting the baseline, detections of trace gases are obtained even though individual features are well below the noise level (*ID5*). IR spectra of 15 drugs of abuse have been analyzed for similarity using techniques of numerical taxonomy. The cluster analysis, principal component analysis, and nonmetric multidimensional scaling elements of the program system NT-SYS were used to structure taxonomic distances between drugs. Ordination diagrams proved to be more visually informative than phenograms (*ID6*).

IR absorption bands in the OH stretching region of the spectrum of phenol in CCl_4 have been analyzed by factor analysis of digitized spectra to detect monomer, linear dimer, and polymeric species (*ID7*). An IR spectrophotometric method for determining the concentration ratio of any two components in multicomponent mixtures has been described. The method is based on a partial regression coefficient ratio, and not only the main peak position but also several other positions in the absorption band are measured. The method is claimed to give about 10-fold enhancement in sensitivity compared with conventional methods (*ID4*).

(IE) Deconvolution of Spectra. Maddams has reviewed the scope and limitations of curve fitting (*B21*), Saltzer has reviewed objectivity of digital band separations (*B148*), and Blass and Halsey have published a book on deconvolution of spectra (*A14*). Fourier transformation techniques have been applied to high resolution laser spectra of water vapor to determine undesirable spectral features. Features such as interference fringes can be mathematically filtered from spectral information in the Fourier domain and the spectral data recovered by an inverse Fourier transformation (*IE1*). A computational method for continuing Fourier spectra using a minimum-negativity constraint, applicable to spectra given by the discrete Fourier transform, has been reported. (*IE2*). A method of determining frequency cutoffs for Fourier domain smoothing by calculation of equivalent widths of narrow peaks in the spectrum has been described (*IE3*). The general theory of Fourier self-deconvolution, i.e., spectral deconvolution using Fourier transforms and the intrinsic line shape of the spectrometer, has been described. The method provides a way of computationally resolving overlapping lines which cannot be resolved due to their intrinsic linewidth. The lines in spectra having a signal/noise ratio $\sim$1000 can readily be reduced in width by a factor of 3 (*IE4*). The deconvolution method of Van Cittert has been used to reliably enhance the effective spectral resolution by a factor of $\sim$3 with data that exhibit a high S/N ($\sim$1000) and in which baseline variations have been eliminated (*IE6*).

A technique has been described for fitting collisional linewidths and shifts from experimental spectral data. The method involves convoluting a low-pressure reference spectrum with a Lorentz function and comparing the convoluted spectrum with higher pressure spectra (*IE5*). The relation between the shape of a true spectrum and that generated by a linear spectrometer can be described by the Fredholm integral equation. Enhancement is limited by overcorrection in the wings of lines and by appearance of negative lobes. The *inherent increase in noise*, caused by the enhancement procedure, can be minimized (*IE7*). A method of estimating values of parameters in models describing positions, widths, and intensities of lines in rotation-vibration bands of gases, without the need for line by line analysis, has been described (*IE8*).

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FOOTNOTES

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