SPECTROMETRY: REPORT OF PANEL

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INTRODUCTION**

In 1981 a workshop was held in Virginia Beach, VA, to assess the role that passive remote sensing might play in tropospheric chemistry. Because the conclusions of that workshop are pertinent to this workshop, they will be summarized, and some data that have become available since that time will be presented. In figure 1 the possible passive remote sensing techniques are summarized. Note that the techniques are split into two viewing geometries--limb viewing and nadir viewing. Since the instrument requirements and capabilities are quite different for the two geometries, the instrument discussion was initially split according to the viewing geometry. It was further split as shown in the figure into radiometry and spectrometry. These categories were further subdivided according to instrument type.

The main advantage of limb viewing is the narrow weighting function (high-altitude resolution) and enhanced sensitivity due to the long atmospheric path. The major disadvantage is the lack of horizontal spatial resolution and, for tropospheric measurements, the probability that clouds in the field of view will limit the amount of data obtained. The geometry of the two paths and the probability of obtaining tropospheric data are shown in figures 2 and 3. Table IV shows the assessment made at the workshop of the potential of the various sensors for long-term measurements. The measurement requirements placed on the sensors at this workshop were fairly stringent as to the spatial coverage desired. Based on this requirement, limb viewing as a possible measurement technique was ruled out and emphasis was placed on nadir viewing. The various nadir-viewing techniques were compared. The results of this comparison are given in table V. Note that this table is based on the constraint of a narrow instrument field of view and an associated rapid detector response. The table gives the advantages and disadvantages of the various sensing techniques and also the technological thrusts needed for the instrument to meet the perceived measurement requirements.

In reviewing these conclusions, one finds that several things have occurred during the intervening period which significantly change some of the conclusions. The first is the realization that the solar occultation technique will yield data on the upper tropospheric distribution of several constituents of interest in tropospheric chemistry. The measurements obtained by the SAGE II satellite (particularly on upper tropospheric water vapor) show that the data are obtained on the tropospheric distribution often enough to give sufficient global coverage to be of interest in tropospheric chemistry. The recent results (Park et al., 1986) obtained by ATMOS, while a much smaller geographic data set, still demonstrated that data are obtained on the upper troposphere often enough to warrant use of such measurement techniques for tropospheric chemistry. When one agrees that limb-viewing geometry

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can be used for tropospheric measurement, then the instrument requirements change, particularly the spectral resolution which is required for the survey-type instrument. Recent results (Murcray et al., 1985) obtained with balloon-borne instruments also illustrate the point. Thus in figure 4, which shows several spectra obtained during sunset from balloon altitude, it is apparant that resolution of ≈0.02 cm^{-1} is required to separate the spectral feature due to F-22 from the interfering absorption due to other compounds. Data concerning the spectral emission from the Earth's limb and also in the nadir-viewing mode have been obtained recently by two groups (University of Denver and Goddard Space Flight Center, Murcray et al., 1983; Murcray, 1984; Goldman et al., 1984; and Kunde et al., 1985). A portion of a limb scan obtained by the University of Denver group is shown in figure 5. This shows the strong emission due to F-12 in the lower stratosphere under this viewing geometry. Figure 6 shows this spectral region under nadir viewing. Note that although the feature is much less prominent, the absorption due to F-12 is clearly identifiable in the spectra. Again, resolution better than 0.1 cm^{-1} is needed to separate spectral features from interferences. These spectra also show the need for high-resolution spectral survey data to be obtained during early satellite missions in order to fully understand the data obtained by species specific instruments.

SOME SPECTROMETRIC TECHNIQUES[†]

Spectroscopic techniques are defined here as those methods which record a continuous portion of the emitted or transmitted spectrum containing spectral features of a number of tropospheric gases of interest; thus, the distinction is made between "species-specific" and "survey" instruments. While this classification may appear to be arbitrary from some points of view, its purpose becomes clearer in the context of the evolution of remote sensing techniques, in which a detailed knowledge of the absorption or emission spectrum is an essential precursor to the design of a species-specific instrument. The spectroscopic instruments of interest here include Grating spectrometers, Fourier Transform spectrometers (usually Michelson interferometers), and scanned Fabry-Perot interferometers.

Once the molecular constituents and the ancillary physical parameters to be measured have been clearly defined, together with their required spatial and temporal coverage, there is a strong motivation to develop methods which are optimized (in terms of the associated data rates) for these specific measurements. In general, spectroscopic techniques are not economic in their use of data transmission and storage systems when they are used to monitor single constituents or physical parameters. Their greatest value is in the early development phase of the program when the detailed spectral environment (i.e., local continuum characteristics, interference from other minor or trace constituents, etc.) must be understood in order that the design of a species-specific instrument and its data analysis procedures can be worked out correctly and with adequate understanding of the details of the radiative transfer in the chosen spectral region.

A question which arises in assessing the role of spectroscopic methods in remote sensing involves consideration of the modes of observation (i.e., limb versus nadir viewing, and emission versus absorption measurements) and the relative merits of the

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[†] Prepared by C. B. Farmer.

available instrumental techniques (e.g., interferometers versus grating spectrometers). A complete discussion of the applicability of these options is beyond the scope of this document; as might be expected, however, each combination of instrument and observing technique has its own range of conditions over which it has superior performance. In general, absorption measurements can only be made in the limb-viewing, solar occultation mode and are thus limited to local sunrise and sunset times; against this they are relatively insensitive to the atmospheric temperature along the line of sight and are capable of high quantitative accuracy. Emission measurements can be made either viewing the atmosphere close to the limb to gain the sensitivity advantage of the long atmospheric paths given by this geometry, or down-looking (near-nadir viewing) to obtain better spatial resolution. Measurements made in emission are more prone to errors associated with uncertainties in the knowledge of the atmospheric temperature along the line of sight. Limb-viewing observations (in both emission and absorption) are capable of better vertical resolution (≈2 km) than are nadir observations (on the order of one pressure scale height); by contrast, the horizontal sampling dimension for limb observations is typically 200 to 300 km, whereas nadir observations can be made in some circumstances with horizontal scales on the order of 10 km.

Recently, several remote sensing spectroscopic techniques have been used successfully to fully record the composition of the troposphere from space, using principally limb-viewing methods (e.g., SAGE and ATMOS); the results have demonstrated the ability to make reliable quantitative determinations of the vertical distributions of both minor and trace constituents. Notable relevant examples include measurements of H_2O vapor, CH_4, N_2O, halogen source species (CFMs, CCl_4, etc.) and aerosols. The ATMOS experiment utilizes a Michelson interferometer in the limb absorption mode; figure 7 illustrates, in bar graph form, the large number of different molecular species seen in the ATMOS data and the altitude ranges over which their concentration profiles can be measured. Figure 8 shows an example of the data for a spectral region which includes an unresolved band of $CFCl_3$ (Freon 11).

While the usefulness of limb-viewing measurements is limited by the presence of tropospheric clouds, the experience gained thus far suggests that measurements in the upper troposphere (i.e., at altitudes above 5 km) are frequently possible, especially at mid-latitudes, and that all altitudes are accessible some of the time. Thus, the often-cited limitation of atmospheric opacity is far outweighed by the proven advantages of the limb-viewing absorption spectroscopy method, its inherent accuracy, good vertical resolution, and the wide range of species that can be measured.

In summary, spectroscopic measurements are required to define the spectral background and provide the detailed spectral information that is essential for the design of species-specific systems and the analysis of data obtained from them. This function of spectroscopic measurements is expected to be an important part of any tropospheric remote-sensing program, and both emission and absorption spectroscopy are relevant in this context. The data from such observations are of value to tropospheric science in their own right, during the initial phases while species-specific techniques and instruments are under development. In addition, there are a number of unresolved problems in tropospheric radiative transfer and spectroscopy (a few examples of which are line mixing in CO_2, line shapes (especially for H_2O), and the behavior of continua) which presently limit the accuracy and reliability of all remote sensing methods. Only through a supporting program of spectroscopic measurements can progress be made in improving our understanding of these aspects of radiative transfer and ultimately reaching the desired confidence in the accuracy of species-specific monitoring techniques.

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TABLE IV.- PASSIVE REMOTE SENSING CONCEPTS

Generic sensor types	Potential long-term measurement roles		Heritage
Species-specific sensors:	Long-term use of proven concepts for selected measurements:		
Optical filter radiometer radiometer	Nadir view:	Profiles of temp., H_2O vapor,	SSH, HIRS
		Burden of ozone, aerosol optical thickness	TOMS, MSS, AVHRR
	Limb view:	Upper trop. profiles of aerosols and ozone	SAM II, SAGE, LIMS
Gas filter radiometer	Nadir view:	Two-layer measurements of CO, CH_4	MAPS
	Limb view:	Upper trop. feasibility TBD	HALOE
Fabry-Perot filter radiometer	Nadir view:	Limited long-term role	CLAES
	Limb view:	Limited long-term role	
Correlation grating spectrometer	Nadir view:	Limited long-term role	COSPEC
Laser heterodyne techniques	Nadir view:	Geosync. orbit } Limited role in penetrating large strat. concentrations to trop. e.g., O_3, HNO_3	IHR
	Limb view:	Geosync. orbit	LHS
Spectral survey sensors:	Preferred long-term concepts for max. measurement capability:		
Grating spectrometer	Nadir view:	Many species and temp. profiles in 3.5- to 15-μm spectral range with spectral resolution of 0.1 cm^{-1} or better	SBUV
	Limb view:		SIRS B
Interferometer	Nadir view:		IRIS
	Limb view:		ATMOS

TABLE V.- COMPARISON OF NADIR-SENSING TECHNIQUES

Type	Advantages	Disadvantages	Technology needs
		Gas filter radiometry	
All types	Low data rate Minimal data reduction High throughput (spectral and angular)	No detailed spectra Limited temperature profiles Test cells limited Species fixed after launch	Gas filter test cells Linear, high-dynamic-range detectors Highly uniform optical elements
		Broadband spectrometry	
All types	Detailed spectral data Survey data Vertical discrimination	High data rate and processing Complex calibration Complex optical train Requires long stability Angle scan	On-board smart processing Cryogenics/cooling
Grating (with linear array)	Simple mechanism	Needs line array for sensitivity Large area gratings	10^3 element arrays Large gratings
Interferometer	High throughput	Background fluctuations Lifetime of high-scan-rate reflector	Mitigation of background fluctuations Multiaperture, multiband interferometer In-flight alignment verification
		Narrow-band spectrometry	
Laser heterodyne spectroscopy	High spectral resolution for vertical discrimination	Limited tuning range	Tunable lasers and heterodyne arrays
Fabry-Perot	Simplicity	Limited tuning range Temperature stability	Improved coatings at long wavelengths

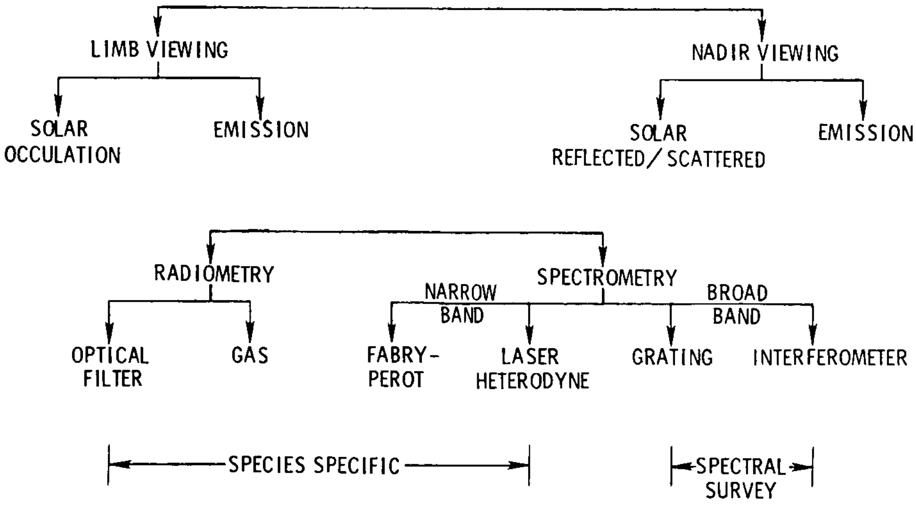

Figure 1.- Passive remote sensing tree showing generic techniques, viewing geometries, and associated sources.

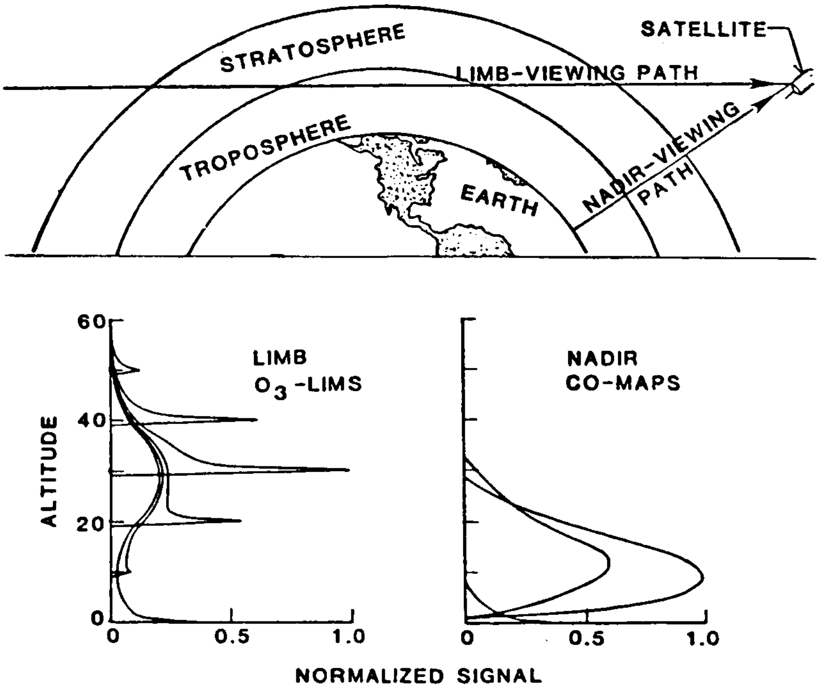

Figure 2.- Comparison of limb and nadir viewing.

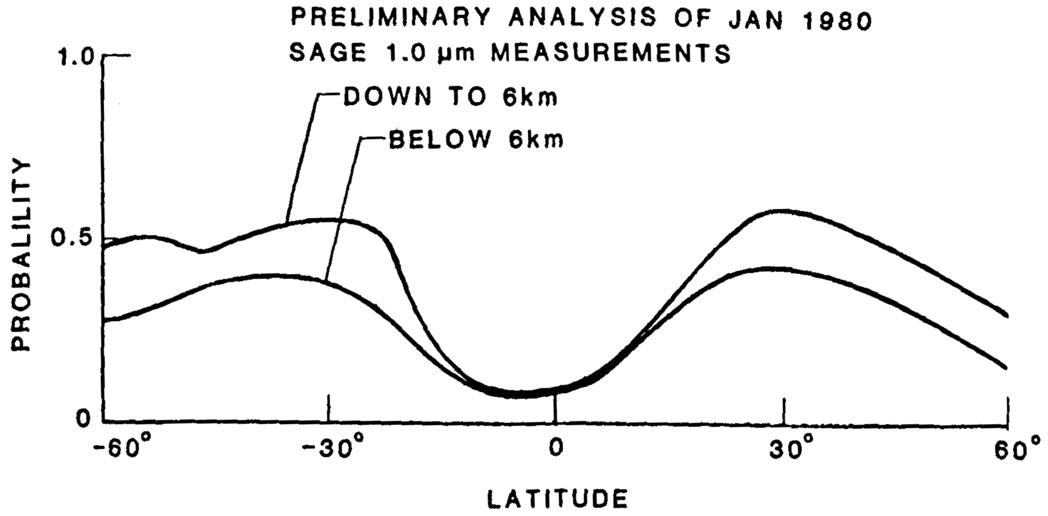

Figure 3.- Probability of limb-viewing measurements in the troposphere.

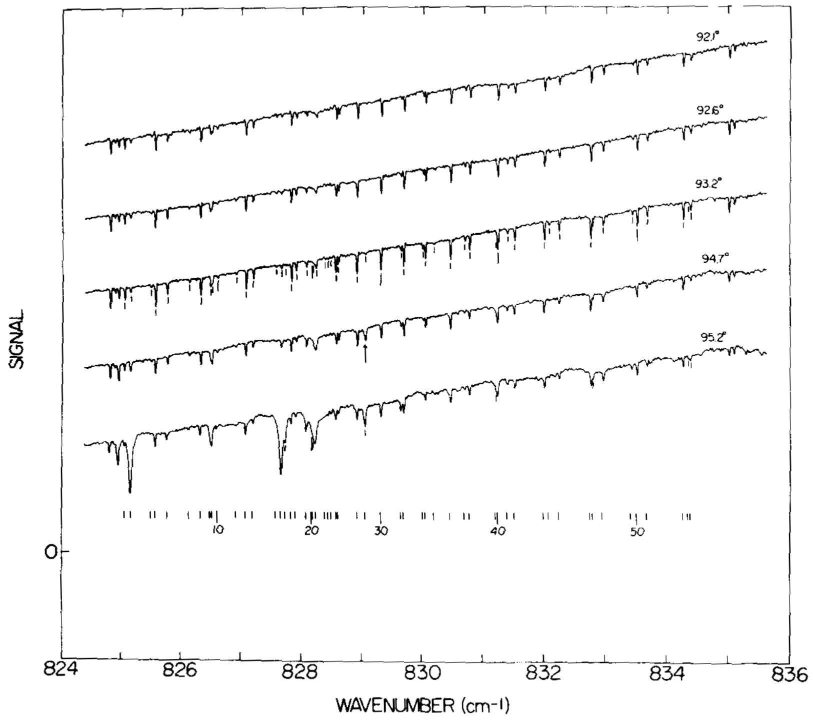

Figure 4.- Solar spectra in the 825-835 cm^{-1} region, obtained during a balloon flight on 23 March 1981, from Holloman AFB, New Mexico, with the University of Denver interferometer system at ≈0.02 cm^{-1} resolution. The altitude and solar zenith angles are indicated on the spectra. Zero levels are offset for clarity. The 829 cm^{-1} F-22 Q-branch is marked with an arrow.

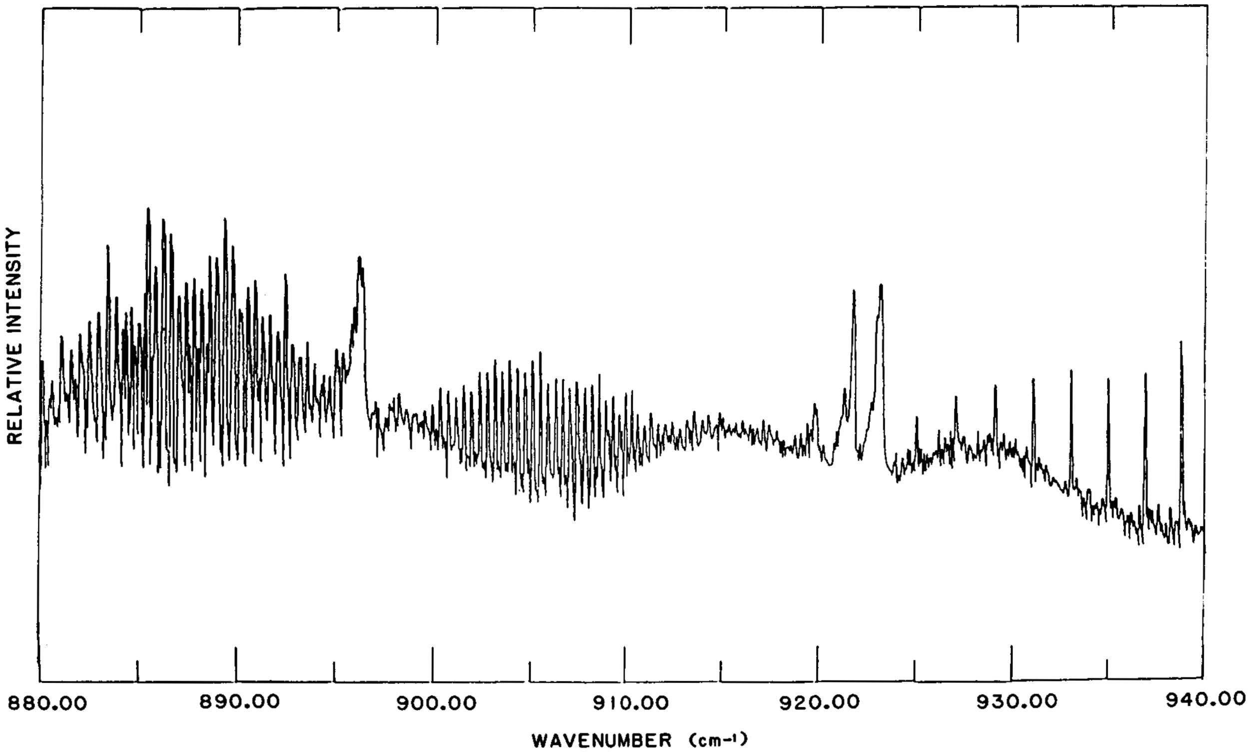

Figure 5.- Atmospheric emission from the Earth's limb as observed from a balloon. Balloon altitude 30 km, viewing angle -3 ½°.

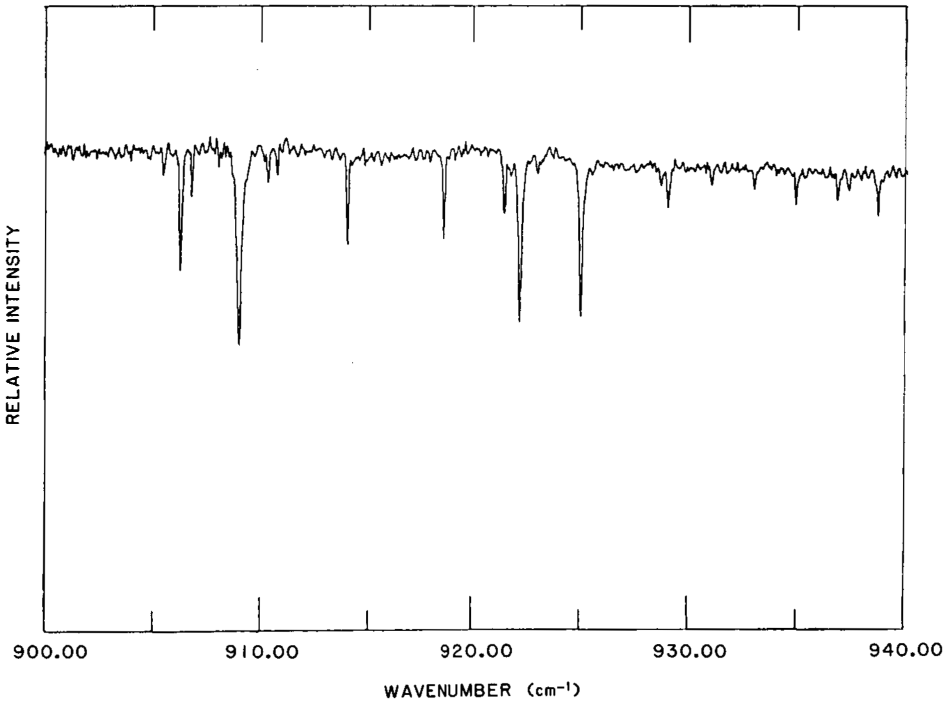

Figure 6.- Earth emission spectra as observed from a balloon at 30 km.

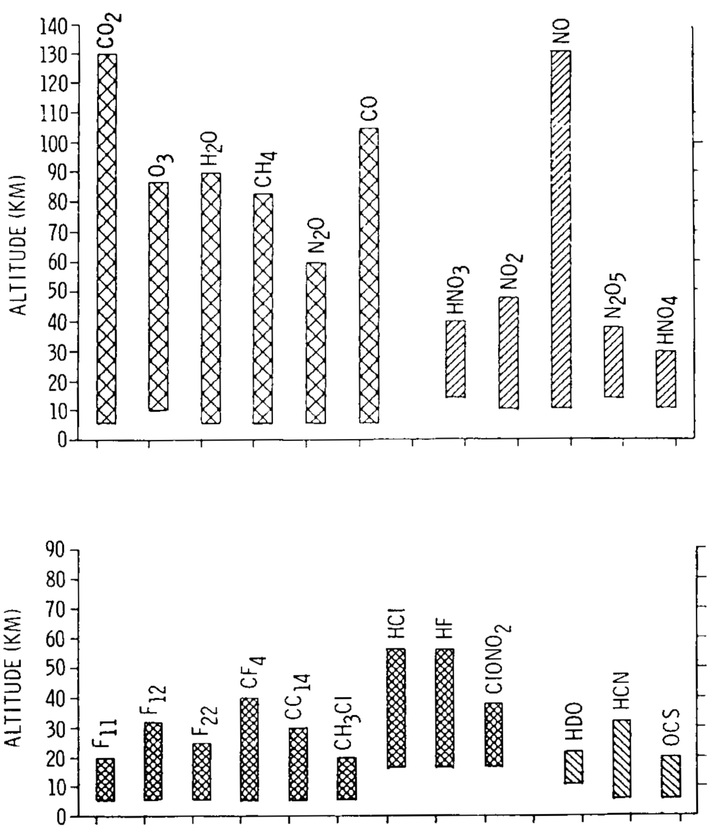

Figure 7.- Atmospheric minor and trace species derived from the ATMOS data, separated into chemical families and indicating the altitude regions over which profiles of concentration have been retrieved.

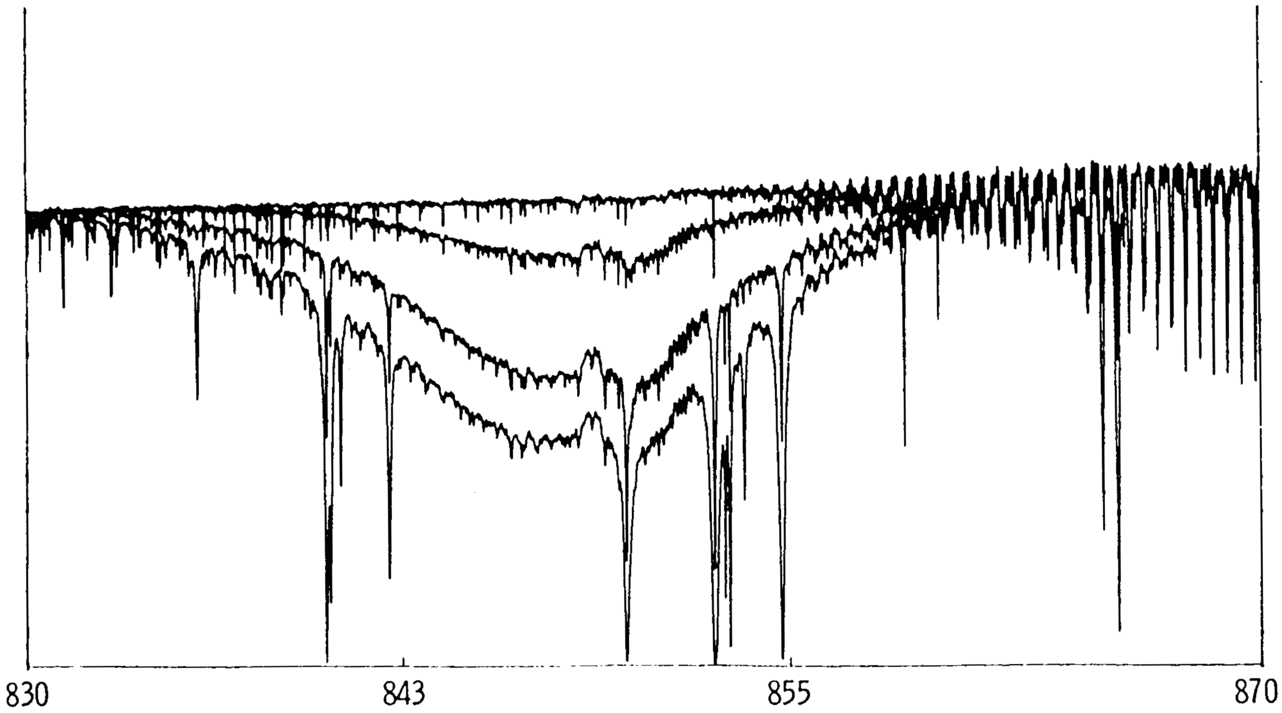

Figure 8.- Portions of four spectra in the region of 830 to 870 cm^{-1} showing large unresolved spectral feature of Freon 11 in the lower three traces which were made at tangent altitudes of 15, 9, and 5 km.