NASA Conference Publication 2396

Review of Spectroscopic Parameters for Upper Atmospheric Measurements

Proceedings of a workshop held at
NASA Langley Research Center
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Edited by
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PREFACE

This report summarizes the informal discussions which took place during the Spectroscopic Parameters Workshop held at NASA Langley Research Center on October 17-19, 1984. A major purpose of this workshop was to review in detail the status of spectroscopic parameters available for atmospheric remote sensing. This type of review had not occurred since the previous Langley workshop in October 1979. In addition, this workshop provided an opportunity for laboratory spectroscopy investigators to understand the spectroscopic parameters requirements of atmospheric remote sensing experiments on the Upper Atmosphere Research Satellite (UARS). These major objectives were accomplished, and the workshop resulted in a series of general and specific recommendations for future laboratory spectroscopy research to meet the needs of UARS and other atmospheric remote sensing programs.

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INTRODUCTION

An informal Spectroscopic Parameters Workshop was held at NASA Langley Research Center, Hampton, Virginia, on October 17-19, 1984. The workshop was initiated as part of the activities of the Spectroscopy Working Group for the Upper Atmosphere Research Satellite (UARS). The objectives of this workshop were:

(1) to communicate UARS spectroscopy requirements to laboratory spectroscopy investigators,

(2) to review the status of current spectroscopic parameters for atmospheric species,

(3) to recommend additional studies.

There were 27 participants in the workshop, including representatives from five UARS experiment teams. Fifteen spectroscopy laboratories, including several from France and England, were represented. A list of attendees appears at the front of this publication.

The workshop began with an overview of the planned UARS mission in 1989, presented by Dr. Aidan Roche, Chairman of the UARS Spectroscopy Working Group. This overview was followed by individual presentations of the specific requirements for the five experiments which use spectroscopic information: CLAES, ISAMS, MLS, HRDI, and HALOE. Summaries of these presentations, including definitions of all acronyms, are given in the first section of this report.

In the second phase of the workshop, a representative of each spectroscopy lab delivered a summary of the work in progress or planned for the near future in his or her laboratory. Many of these summaries highlighted unique facilities or special capabilities at individual labs. These presentations are discussed in Section 2.

The third segment of the workshop consisted of a detailed review of the status of spectroscopic parameters for atmospheric remote sensing, as they are currently available in the AFGL (Rothman et al., 1983a,b) and GEISA (Husson et al., 1985) compilations. Dr. Larry Rothman of AFGL reviewed the status of the parameters for each molecule listed in the present (1982) version and discussed updates that are planned for the new version to be released in mid-1985. Dr. Nicole Husson discussed the differences between the present versions of the GEISA and AFGL compilations, reviewing in detail the recent addition, initiated by A. Chedin, of new parameters for the temperature dependence of the air-broadened halfwidths for a number of atmospheric species. Presentations given by Dr. Linda Brown of JPL and Dr. Aaron Goldman of the University of Denver used high-resolution atmospheric and laboratory spectra to illustrate the need for further improvements in the spectroscopic data bases. These reviews are summarized in Section 3 of this report.

The workshop ended with an open discussion covering a wide range of topics including the future status and proposed changes in the format of the spectroscopic data compilations, timetables for inclusion of new spectroscopic parameters in UARS data reduction, and mechanisms for funding UARS-related spectroscopic research. A summary of this discussion is given in Section 4 of this report, along with general and specific recommendations for future studies.

1. UARS SPECTROSCOPIC REQUIREMENTS

The Upper Atmosphere Research Satellite (UARS), scheduled to be carried into low Earth orbit (600 km) in the fall of 1989, carries 10 experiments designed to monitor the condition of the Earth's upper atmosphere over a 2-year period. The measurements to be performed fall into three general categories: (1) composition and structure, (2) winds, and (3) energy input. Table 1.1 lists the names and acronyms for these individual experiments. A more detailed description of the UARS satellite and its mission is available in a separate report (Reber, 1985).

Five of the UARS experiments, including all of those designed to measure composition and structure, use spectroscopic techniques to obtain the desired measurement. Wavelengths employed range from the microwave to the visible. Figures 1.1 and 1.2 summarize the molecules, altitude ranges, and spectral regions to be observed by these five experiments. The UARS Spectroscopy Working Group has been charged with the task of evaluating the presently available spectroscopic line parameters (positions, intensities, halfwidths, line shapes and their temperature dependence) used in the development of data reduction algorithms and in the modeling of instrument performance. The working group is also responsible for recommending additional laboratory spectroscopy studies to provide appropriate new data for molecules and spectral regions where existing line parameters are inadequate for UARS experiments. To this end, the working group is compiling a Spectroscopy Requirements document which describes in detail the specific accuracy requirements for spectroscopic parameters needed by the individual UARS experiments. This document will be circulated to major spectroscopy laboratories in 1985 to encourage research directed toward meeting UARS requirements.

Examples of specific requirements in selected spectral regions are given in the following few paragraphs:

CLAES. This experiment measures thermal emission from the Earth limb using a Fabry-Perot interferometer and several interference filters. Interfering emission by HNO_3 and O_3 is a problem in several of the CLAES filter regions, particularly the $CFC\ell_3$ and aerosol filter at 835-845 cm^{-1} and the CH_4 and N_2O filter at 1288-1294 cm^{-1}. Within these regions, line center positions for both HNO_3 and O_3 are needed within $\pm$ 0.001 cm^{-1}; band intensities accurate to $\pm$ 3 percent and relative line intensities accurate to $\pm$ 1 percent are also needed for these two species. Pressure and temperature retrievals for CLAES will be performed using emission measurements in the CO_2 Q-branch near 792 cm^{-1}. CO_2 and O_3 band intensities accurate to $\pm$ 3 percent and relative line intensities accurate to $\pm$ 1 percent are required in this region.

High-quality characterization (e.g. absorption coefficients or band model parameters) is also needed for several broad features. These include the vibration-rotation bands of $CF_2C\ell_2$ near 921 cm^{-1} and $CFC\ell_3$ in the 735-745 cm^{-1} region, as well as the collision-induced fundamental band of O_2 in the 1600-1610 cm^{-1} region. Absorption in the far wings of lines belonging to H_2O, CO_2, and O_3 bands between 800 and 1200 cm^{-1} must also be accurately determined.

ISAMS. This experiment has conventional radiometer channels for measuring HNO_3 and O_3 and both conventional and Pressure Modulated Radiometer (PMR) channels for measuring temperature (CO_2), H_2O, N_2O, CH_4, CO, NO, and NO_2. The channels are typically 50 to 100 cm^{-1} wide, so that accurate parameters for many spectral lines are required for the retrieval calculations. Since the PMR cells contain pure samples of the target gas at pressures up to approximately 30 torr, self-broadened halfwidths and line shapes are needed in addition to the air-broadened parameters. The accuracy of the line parameters affects the accuracy of the retrieved atmospheric species concentration. For example, computer simulations show that to achieve a 2-percent absolute accuracy in the retrieved CO concentration from PMR measurements at 2050-2250 cm^{-1}, CO line intensities are needed to ± 11 percent, air-broadened halfwidths to ± 2.3 percent, and self-broadened halfwidths to ± 6.2 percent. The accuracy requirements for line parameters are a function of the tangent height of the measurement; the numbers given here are worst-case values. Similarly, in the CH_4 channel at 1340-1460 cm^{-1}, CH_4 line intensities are needed to ± 6 percent, air broadened halfwidths to ± 2.5 percent, and self-broadened halfwidths to ± 2.3 percent. It is expected that similar accuracies will be required for line parameters in other PMR channels. Since ISAMS is an emission radiometer, very good temperature measurements are needed; these measurements require very accurate knowledge of the CO_2 line parameters in the 15-μm region. Accurate line parameters are also required for species such as O_3, HNO_3, H_2O, CH_4, and CO_2 where their atmospheric signals interfere with the signal from the target gas.

MLS. Gas concentration retrievals of H_2O, O_3, H_2O_2, and $C\ell O$ for MLS are based on least-squares fits to high resolution microwave measurements of single spectral lines. Because the results are very dependent on the line shapes, it is important to have very accurate (1 to 2 percent) air-broadened halfwidth values for the target lines over the range of temperatures encountered in the upper atmosphere, 190-300 K. Line parameters for interfering gases in these narrow spectral regions are also needed.

HRDI. This experiment will obtain upper atmospheric wind profiles from inversion of the shapes of several individual O_2 lines belonging to the A, B, and γ bands in the 6300-7000Å region. Required parameters for these lines include intensities, halfwidths and their temperature dependence, pressure-induced line shifts, and line shapes, especially in the far wings. Parameters are needed for all the isotopic variants of O_2.

HALOE. This instrument will determine concentrations of several key species involved in ozone chemical cycles by measuring atmospheric absorption of solar radiance during occultations at sunrise and sunset. There are four gas correlation channels to measure HF, $HC\ell$, CH_4 and NO, and four radiometer channels to measure NO_2, H_2O, O_3, and atmospheric pressure (CO_2). Each of the correlation cells is filled with a relatively high concentration (e.g., 10 percent for $HC\ell$, 50 percent for HF) of the target gas in N_2 at typical pressures of 0.1 atm. Therefore, in addition to air-broadened halfwidths, accurate self-broadened and N_2-broadened halfwidths are required for the 1-0 bands of HF, $HC\ell$, and NO and the ν_3 band systems of CH_4. Accuracy requirements for all parameters have been determined in instrument simulation studies, and they are briefly summarized in Table 1.2. High-priority requirements include intensities, halfwidths, and line shapes in the 1-0 bands of HF and $HC\ell$; CH_4 halfwidths and their temperature dependence in the 2.5-μm,

Table 1.1 UARS Experiments

Composition and Structure

CLAES - Cryogenic Limb Array Etalon Spectrometer

HALOE - Halogen Occultation Experiment

ISAMS - Improved Stratospheric and Mesospheric Sounder

MLS - Microwave Limb Sounder

Winds

HRDI - High Resolution Doppler Imager

WINDII - Wind and Temperature Remote Sensor II

Energy Input

SOLSTICE - Solar Stellar Irradiance Comparison Experiment

SUSIM - Solar UV Spectral Irradiance Monitor

PEM - Particle Environment Monitor

ACRIM - Active Cavity Radiometer Irradiance Monitor

Table 1.2 HALOE Accuracy Requirements for Spectral Line Parameters

Parameter	Target Gas	Interfering Gases
Line positions	± 0.001 cm^{-1}	± 0.001 cm^{-1}
Line intensities	± 2% strong lines ± 5% weak lines	± 3% strong lines ± 10% weak lines
Collision broadened Halfwidths	± 3% strong lines ± 10% weak lines	± 5% strong lines ± 20% weak lines

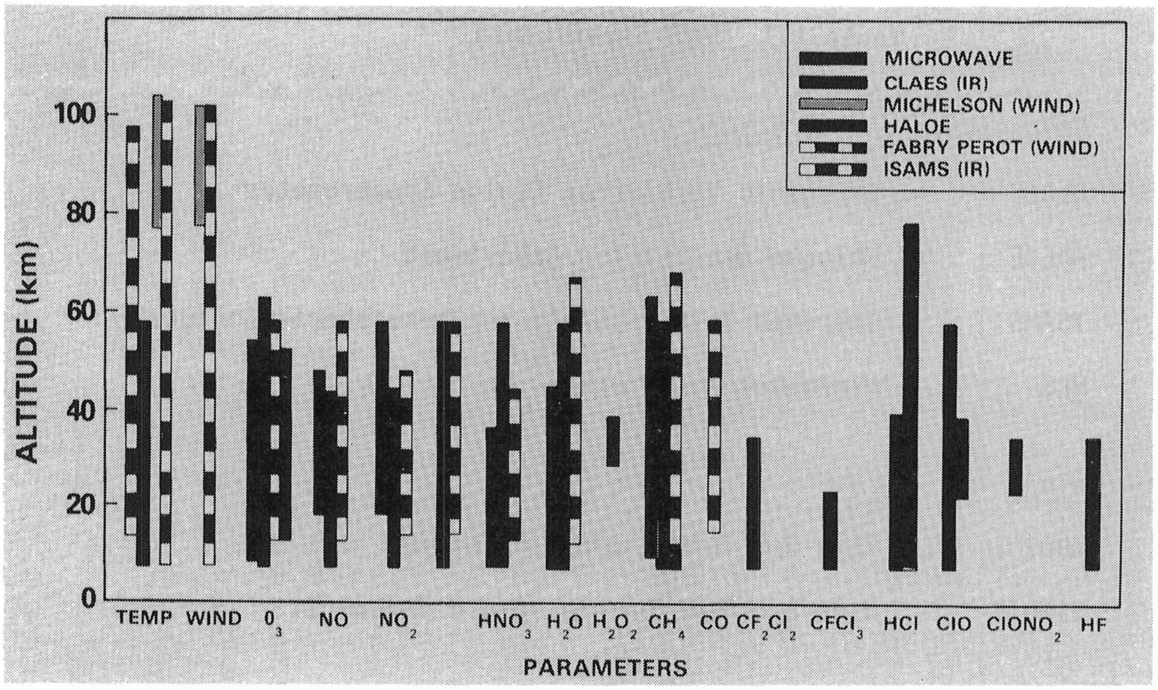
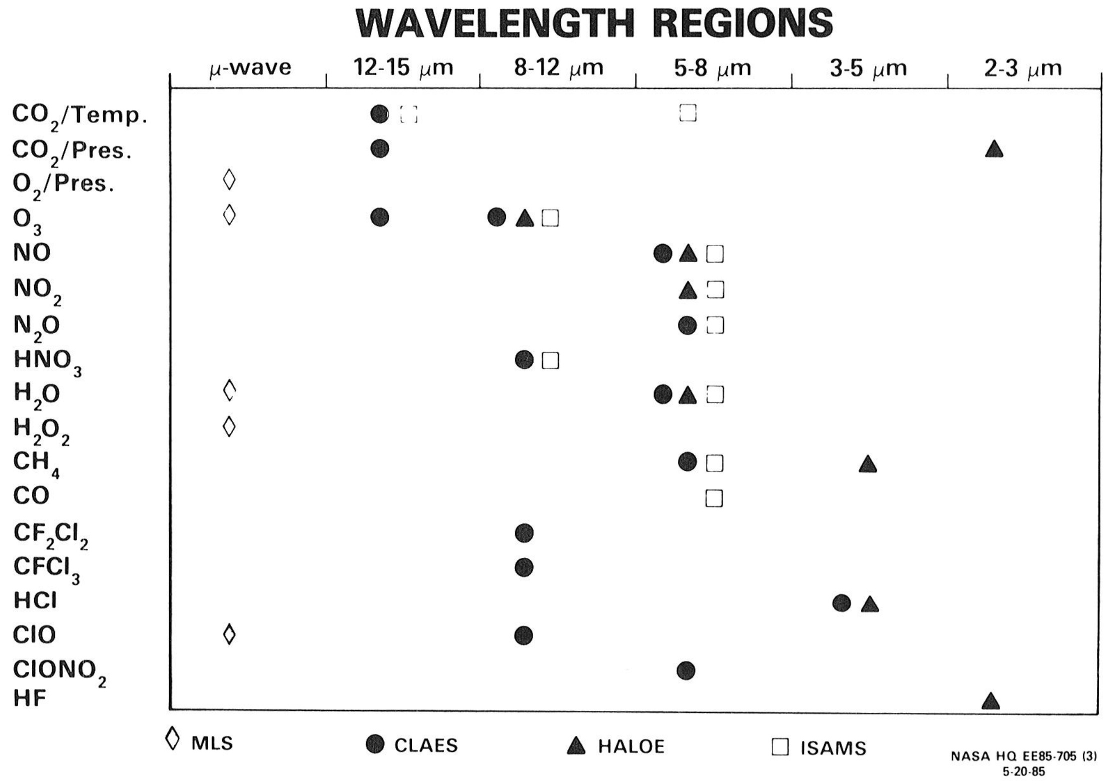


Figure 1.1 UARS remote atmospheric sensors.



WAVELENGTH REGIONS

	μ-wave	12-15 μm	8-12 μm	5-8 μm	3-5 μm	2-3 μm
CO_2/Temp.		● □		□		
CO_2/Pres.		●				▲
O_2/Pres.	◊					
O_3	◊	●	● ▲ □			
NO				● ▲ □		
NO_2				▲ □		
N_2O				● □		
HNO_3			● □			
H_2O	◊			● ▲ □		
H_2O_2	◊					
CH_4				● □	▲	
CO				□		
CF_2Cl_2			●			
$CFCl_3$			●			
HCl					● ▲	
ClO	◊		●			
$ClONO_2$				●		
HF						▲

◊ MLS ● CLAES ▲ HALOE □ ISAMS

Figure 1.2 UARS temperature and constituent measurements.

3.5-μm, and 6- to 8-μm regions; more accurate absorption coefficients for the collision-induced fundamental band of O_2, in the typical atmospheric range of pressure and temperature; improved line positions and intensities for O_3 in all spectral regions; improved line parameters for CO_2 in the 2.7-μm region; and temperature dependence of halfwidths for all target and interfering species.

The five UARS experiments mentioned above represent a diverse group of measurement techniques, each having specialized requirements for accuracy in line parameters. However, there are some general requirements which appear to be common to most of these experiments. These are: infrared line positions accurate to ± 0.001 cm^{-1}, line intensities with 2-percent to 5-percent absolute accuracy, air-broadened halfwidths for all species, and self-broadened halfwidths for certain target species with 1-percent to 5-percent accuracy over the range of temperatures to be encountered in the atmosphere or in the instrument environment. A detailed description of all the UARS spectroscopic requirements for the individual experiments is being compiled by the Spectroscopy Working Group (A. Roche, chairman).

2. CURRENT LAB SPECTROSCOPY EFFORTS AND CAPABILITIES

The spectroscopy laboratories represented at the workshop contain a wide range of instruments with differing resolution and specialized absorption cells. The majority of these labs use either high-resolution Fourier transform spectrometer (FTS) or tunable diode laser (TDL) systems to record spectral data. Some labs use both types of systems in the same study, taking advantage of the wide spectral coverage and wavenumber precision of the FTS and the high resolution and radiometric accuracy of the TDL. Other types of spectrometers in use include large grating spectrometers, a difference-frequency laser spectrometer, and heterodyne systems using various types of lasers as local oscillators.

Many of the absorption spectroscopy experiments are performed using "ordinary" glass cells with salt or sapphire windows. Special metal cells have been constructed for measurements of corrosive gases such as HCℓ or HF. Coolable cells of either metal or glass have been used in intensity measurements and in studies of the temperature dependence of halfwidths. White cells are useful for measurements of intensities in complex band systems, allowing long absorption paths, but minimizing pressure broadening so that individual lines can be resolved. Some recently constructed or planned White cells are coolable, and a few are also capable of containing corrosive gases. Finally, there are a few ongoing programs, notably at the University of Denver, NCAR, and Kitt Peak, which regularly obtain atmospheric spectra with absorption paths longer than are presently obtainable in any laboratory. Specific information on the capabilities of the various laboratories is given in Table 2.1.

Table 2.2 summarizes current laboratory spectroscopy studies, including results which were complete but not published by mid-1984, work in progress at the time of the workshop, and studies planned to get under way before the end of 1985. The majority of these current efforts are directed toward the accurate determination of line positions, assignments, and intensities for many absorption bands of major infrared-active atmospheric constituents (H_2O, CO_2, O_3, N_2O, CH_4) and their isotopic variants. There are also a number of current efforts to measure self-broadened, N_2-broadened, or air-broadened

Table 2.1 Special Capabilities for Laboratory Spectroscopy

Labs	Instrument (Resolution)	Cells
AFGL Optics Division	2-m FTS (0.005 cm^{-1})	3 m heatable cell
CNRS Lab.d'Infrarouge, Orsay	Guelachvili FTS (0.0025 cm^{-1} unapodized, 0.005 cm^{-1} apodized) TDL (0.001 cm^{-1})	Short cryogenic cells: 1, 10, 30 cm coolable to 200K Cryogenic White cell 1 m base path, ≈ 40 m max coolable to 200K
JPL	Microwave spectrometer TDL (0.001 cm^{-1})	
Los Alamos	2-1/2 m FTS (0.002 - 0.001 cm^{-1}) National Facility to become available in 1986	
NASA Ames	Bomem FTS (0.004 cm^{-1}) TDL (0.001 cm^{-1}) Nicolet FTS (0.06 cm^{-1})	Several short cryogenic cells ≤ 30 cm White cells 0.75 m base path, ≈ 35 m max 25 m base path, ≈ 3 km max Cryogenic White cells (future) 2 m base path gold-coated interior
NASA Goddard	TDL (0.001 cm^{-1}) CO_2 laser heterodyne	
NASA Langley	TDL (0.001 cm^{-1}) Nicolet FTS (0.06 cm^{-1})	5, 10, 25, 50 cm glass cells 50 cm glass coolable cell 10 cm sealed gold cells (HALOE)
NBS Boulder	Heterodyne systems for frequency measurements	
NBS Gas and Particulate Div.	Nicolet FTS (0.06 cm^{-1})	
NBS Molecular Spectroscopy Div.	Difference-frequency laser TDL spectrometer (0.0001 cm^{-1}) TDL systems (0.001 cm^{-1}) Bomem FTS (0.004 cm^{-1})	Coolable cell
NCAR	FTS (0.02 cm^{-1})	Atmospheric spectra from aircraft
NOAA/NESDIS	TDL (0.001 cm^{-1}) Vacuum grating spectrometer	8 m coolable cell
NSO/Kitt Peak	Brault FTS (0.01 - 0.005 cm^{-1})	White cell, room temperature ≈ 384 m max effective path Ground-based atmospheric spectra (monthly)
Rutherford Appleton Labs	Bomem FTS (0.004 cm^{-1})	3 mm, stainless steel 5 cm, stainless steel coolable to 200 K White cell, stainless steel coolable to 200 K 40 cm base path, ≈ 20 m max White cell, stainless steel, coolable to 200 K, 8 m base path, ≈ 1 km max
University of Denver	He-cooled grating spectrometers (0.3 cm^{-1}) Eocom FTS (0.06 cm^{-1}) Bomem FTS (0.02 cm^{-1}) Bomem FTS (0.004 cm^{-1}) He-cooled interferometer (0.1 cm^{-1})	Laboratory coolable cells Ground, aircraft, and balloon atmospheric spectra (≈ 4 flights per year)
Universite de Reims	SISAM (0.02 cm^{-1}) Stepping FTS (0.003 cm^{-1})	4 m coolable cell 3 m room temperature cell

Table 2.2 Current Laboratory Spectroscopy

Molecule	Spectral coverage (cm^{-1})	Band(s)	Instrument and resolution	Data type	Status*	Accuracy	Source
H_2O		Ground state			P		JPL (Poynter)
H_2O		Ground state		Halfwidths	U		JPL (Pickett, Cohen)
H_2O	1000-5000	$\Delta K_a = 1$ line		Intensities	U		JPL (Brown, Toth)
H_2O	1000-2000			Positions	C	For calibration	JPL (Brown, Toth)
H_2O	10 000-25 000				U		JPL (Toth)
HDO		Ground state			P		JPL (Poynter, Toth)
HDO	500-2000	ν_2 and hot bands	FTS 0.0006 cm^{-1}	Positions, assignments	U	0.0004 cm^{-1}	AFGL/Utah State (Esplin, Rothman)
HDO	≈ 1600			Positions, intensities	C		JPL (Toth)
CO_2	700-1100				U		JPL (Brown, Toth)
CO_2	700-750	$10^00 \leftarrow 01^10$	TDL	Intensities, halfwidths (self and N_2)	U	5% 5%	Lab. d'Infrarouge (Huet, Lacome, Levy)
CO_2	900-1000	$00^01 \leftarrow 01^00$	CO_2 laser absorption spectroscopy	Halfwidths (self, N_2, O_2) with T-dependence	P	3% to 5%	Lab d'Infrarouge (Arie, Arcas, Lacome, Levy)
CO_2 asymmetric isotopes	≈ 1430	8 bands		Positions, intensities	C	0.0004 cm^{-1} 3% to 7%	JPL (Toth)
$^{13}O^{16}O^{18}O$	2086-2307	$\Delta\nu_3 = 1$, Σ-Σ and π-π type	FTS 0.005 cm^{-1}	Positions, assignments	C	0.0005 cm^{-1}	Lab. d'Infrarouge (Bailly, Rossetti)
CO_2 and isotopes	1900-4000	14 bands near 2200 cm^{-1} 23 bands near 3600 cm^{-1}	FTS 0.006 cm^{-1}	Positions, assignments	C	0.0004 cm^{-1}	AFGL/Utah State (Esplin, Rothman)
CO_2 and isotopes	1800-2600	≈ 60 bands	FTS 0.01 cm^{-1}	Positions, assignments, intensities	C P	0.0004 cm^{-1} 2% strong lines 50% weakest lines	NASA Langley (Rinsland, Benner, Malathy Devi)
CO_2 and isotopes	3100-4100	Many	FTS 0.01 cm^{-1}	Positions, assignments, intensities	P P	0.0004 cm^{-1}	NASA Langley (Rinsland, Benner, Malathy Devi)
O_3	Microwave	ν_2, $2\nu_2$ states			P		JPL (Cohen, Pickett)
O_3	Microwave			Halfwidths	U		JPL (Pickett, Cohen)
O_3	600-800	ν_2	FTS 0.005 cm^{-1}	Positions, assignments, relative intensities	P	0.0004 cm^{-1}	NASA Langley (Rinsland, Smith, Malathy Devi, Barbe, Goldman)
O_3		ν_2			U		JPL (Pickett, Cohen)
O_3	≈ 1000 cm^{-1}	ν_1, ν_3		Positions, assignments, intensities	C		JPL (Pickett, Cohen, Margolis)
O_3	970-1100	ν_1, ν_3	TDL	Halfwidths (air) with T-dependence	P		NASA Langley (Smith, Malathy Devi, Rinsland,
O_3	600-5000	All	FTS 0.005 cm^{-1}	Survey spectra 9.6 μm Positions, intensities, halfwidths (air) with T-dependence	U	0.0005 cm^{-1} 5% 3%	RAL (Ballard, Gunson)
$^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$	Microwave	ν_2 state		Positions	C		JPL (Chiu, Cohen)
$^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$	950-1400	ν_1, ν_3	FTS 0.005 cm^{-1} TDL	Positions, assignments, intensities	P	0.0004 cm^{-1}	NASA Langley (Smith, Malathy Devi, Rinsland, Hoell, Flaud, Camy-Peyret)

*C = Complete but not published by mid-1984; P = in progress; and U = Under way in 1985.

Table 2.2 Continued

Molecule	Spectral coverage (cm^{-1})	Band(s)	Instrument and resolution	Data type	Status*	Accuracy	Source
$^{16}O^{16}O^{17}O$ and $^{16}O^{17}O^{16}O$		Rotational		Positions			JPL (Cohen, Pickett, Hillig)
N_2O	500-700	ν_2 and hot bands	FTS 0.005 cm^{-1} TDL	Positions, assignments, intensities	P	0.0002 cm^{-1} 10%	NBS/Univ. of Oulu (Maki et al.)
N_2O	≈ 900	ν_1, ν_3		Positions, intensities	C		JPL (Toth)
N_2O	900-2000	Many		Positions	C	For calibration	JPL (Brown, Toth)
N_2O	≈ 1100 cm^{-1}	All		Positions, intensities	C		JPL (Toth)
N_2O	1100-1110 and 1830-1950	$2\nu_2$, $\nu_1 + \nu_2$, and hot bands	FTS 0.005 cm^{-1} TDL	Positions, assignments, intensities	C	0.0002 cm^{-1} 10%	NBS/Univ. of Oulu (Maki et al.)
N_2O	≈ 2000 cm^{-1}	All		Positions, intensities	C P		JPL (Toth)
N_2O	≈ 2500 cm^{-1}	All		Positions, intensities	C		JPL (Toth)
N_2O	2850-3330	All		Positions, Intensities	P		JPL (Toth)
N_2O	≈ 4550 cm^{-1}	All			U	JPL (Toth)	
CO	≈ 2000 cm^{-1}	1-0		Positions	C	For calibration	JPL (Brown, Toth)
CH_4	≈ 1400 cm^{-1}	ν_2, ν_4 and hot bands			P		JPL (Brown, Hilico, et al.)
CH_4 and isotopes	1100-1450	ν_4	FTS 0.01 cm^{-1} TDL	Halfwidths (N_2 and air) T-dependence	P U	3%	NASA Langley (Malathy Devi, Smith, Rinsland)
CH_4	1100-1500	ν_4	FTS 0.005 cm^{-1}	Positions, intensities, halfwidths (air) with T-dependence halfwidths (self)	P	0.0005 cm^{-1} 5% 3% 3%	RAL (Ballard)
CH_4	≈ 1800 cm^{-1}	$\nu_3 - \nu_4$			C		JPL (Hilico, Loete, Brown)
CH_4	≈ 4350 cm^{-1}			Assignments	P		JPL (Brown, Hilico, et al.)
CH_4 and isotopes	≈ 4500 cm^{-1}	All		Positions	C		JPL (Brown)
CH_4	≈ 6250 cm^{-1}	$2\nu_3$			U		JPL (Margolis)
O_2	Microwave	Singlet-delta rotational			C		JPL (Hillig, Chiu, Reed, Cohen)
NO		Rotational $v = 0$; $v = 1$			P		JPL (Pickett, Cohen)
NO	1800-2000	1-0	FTS 0.005 cm^{-1}	Positions, intensities, halfwidths (air) with T-dependence halfwidths (self)	U	0.0005 cm^{-1} 5% 3% 3%	RAL (Ballard
NO	3700-3880	2-0	Difference-freq. laser spectrometer 0.0001 cm^{-1}	Intensities, halfwidths (self), and shapes	C	1% 2%	NBS (Maki, Pine)
NO_2	≈ 1600 cm^{-1}	ν_3 and hot bands			P		JPL (Toth)
NH_3	≈ 900 cm^{-1}	ν_2		Positions	C		JPL (Margolis, Poynter)
NH_3	≈ 1500 cm^{-1}	ν_4		Ground state constants	C		JPL (Cohen, Weber, Poynter, Margolis)
NH_3	≈ 1600 cm^{-1}	ν_4, $2\nu_2$			P		JPL (Poynter, Margolis)

*C = Complete but not published by mid-1984; P = in progress; and U = Underway in 1985.

Table 2.2 Concluded

Molecule	Spectral coverage (cm^{-1})	Band(s)	Instrument and resolution	Data type	Status*	Accuracy	Source
HNO_3	1240-1370	ν_3, ν_4	FTS 0.005 cm^{-1}	Positions, assignments	P	0.002 cm^{-1}	RAL (Gunson)
HNO_3	850-925 1280-1345 1675-1740	ν_5, $2\nu_9$ ν_3, ν_4 ν_2	FTS 0.005 cm^{-1} TDL	Positions, assignments, intensities	P	0.001 cm^{-1} 20%	NBS/Univ. of Denver (Maki, Goldman, et al.)
OH and OD		Rotational			U		JPL (Pickett et al.)
HF	3500-4300	1-0	Difference-freq. laser spectrometer 0.0001 cm^{-1}	Intensities, halfwidths (self and N_2), lineshapes	C P P	1% 1% 1%	NBS (Pine)
$HC\ell$	2600-3100	1-0	FTS 0.06 cm^{-1}	Halfwidths (HF-broadening)	C	10%	NASA Langley (Smith, et al.)
$HC\ell$	2650-3080	1-0	FTS 0.01 cm^{-1} and 0.005 cm^{-1}	Intensities, halfwidths (self and N_2) with T-dependence	C C	4% 2%	NASA Ames (Chackerian, Goorwitch, Giver)
$HC\ell$	2700-3050	1-0	Difference-freq. laser spectrometer 0.0001 cm^{-1}	Intensities, halfwidths (self and N_2), lineshapes	C P P	1% 1% 1%	NBS (Pine)
OCS	839-887	ν_1	TDL 0.001 cm^{-1}	Halfwidths (N_2-broadening) (self-broadening)	C P	5%	Lab. d'Infrarouge (Bouanich)
OCS	490-560 800-890 1010-1090 1650-1740 1845-1920	ν_2 ν_1 $2\nu_2$ $2\nu_1$ $\nu_1 + 2\nu_2$ and hot bands	FTS 0.005 cm^{-1} TDL	Positions, assignments, intensities	C	0.0002 cm^{-1} 10%	NBS/Univ. of Oulu (Maki et al.)
H_2CO	≈ 1800 cm^{-1}	ν_2			P		JPL (Brown)
HCN	3200-3400	ν_3	FTS 0.06 cm^{-1}	Halfwidths (HF-broadening)	C	10%	NASA Langley (Smith et al.)
C_3H_8 (propane)	500-4000		FTS 0.06 cm^{-1}	Band centers, band intensities, and T-dependence	U	0.02 cm^{-1} 3% to 5%	NBS (Elkins)
$CC\ell_3F$ (F-11)	700-1200		FTS 0.06 cm^{-1}	Band centers, band intensities, and T-dependence	U	0.02 cm^{-1} 3% to 5%	NBS (Elkins)
$CC\ell_2F_2$ (F-12)	700-1200		FTS 0.06 cm^{-1}	Band centers, band intensities, and T-dependence	U	0.02 cm^{-1} 3% to 5%	NBS (Elkins)
$CH_3CC\ell_3$ (methyl chloroform)	700-1200		FTS 0.06 cm^{-1}	Band centers, band intensities, and T-dependence	U	0.02 cm^{-1} 3% to 5%	NBS (Elkins)
HNO_2	1240-1280	ν_3 (trans-HNO_2)	TDL	Positions, assignments, intensities	C	0.001 cm^{-1} 10%	NBS (Maki)
NO_3	mid-IR Visible	Several	FTS 0.05 cm^{-1}	Band identification	P		RAL (Wassell)
Numerous species	600-3100	Many	FTS 0.06 cm^{-1} and 0.02 cm^{-1}	Reference spectra, Some absorption coefficients	C		Univ. of Denver (Goldman)

*C = Complete but not published by mid-1984; P = in progress; and U = Under way in 1985.

halfwidths. Many of these studies also involve measurements of the temperature dependence of the halfwidths and measurement of non-Lorentzian line shapes. Some of the studies included in the table were initiated to meet line parameter requirements of current atmospheric remote sensing experiments such as those involved in the Balloon Intercomparison Campaign of 1982/83 and the ATMOS experiment on Spacelab 3 in 1985. However, these laboratory spectroscopy results will also be of benefit to UARS.

3. STATUS OF CURRENT SPECTROSCOPIC PARAMETERS

The AFGL and GEISA line parameter compilations serve as the spectroscopic data base for most atmospheric remote sensing efforts in North America and Europe. The AFGL compilations began in 1973 with parameters for only the seven "major gases" (H_2O, CO_2, O_3, N_2O, CO, CH_4, and O_2), and have since expanded to include a "trace-gas" compilation. Presently the AFGL compilations include parameters for a total of 28 gases, and updates are released at intervals of approximately 2 years. Details of the updates are published in a number of articles in Applied Optics by L. S. Rothman and collaborators (see Rothman et al., 1983a,b). The GEISA compilation began in 1976 and has most of its data in common with the AFGL compilations. It is also updated at intervals of approximately 2 years, but these do not occur simultaneously with the AFGL updates. The GEISA updates are documented in a series of reports by A. Chedin, N. Husson, and co-workers at the Laboratoire de Meteorologie Dynamique du C.N.R.S. in France (see Husson et al., 1985). A list of gases whose parameters are in the present AFGL compilations is given in Table 3.1. The table also lists other molecules of interest for the terrestrial atmosphere which may be included in future updates of the compilations as line parameters become available. Some of these gases (e.g., C_2H_4) are already included in the GEISA compilation. A catalog of over 200,000 microwave and submillimeter transitions for 151 different gases is also maintained at JPL (Poynter and Pickett, 1980, 1981, 1984). Many of these data have also been incorporated into the AFGL and GEISA compilations. Other less comprehensive compilations of spectroscopic data are also useful for atmospheric remote sensing. Two recent examples are the collections of high-resolution laboratory reference spectra produced at the University of Denver (Murcray and Goldman, 1981; Murcray et al., 1984), and the bibliographic tables of band intensities and broadening parameters contained in two volumes of the Molecular Spectroscopy: Modern Research series (Pugh and Narahari Rao, 1976; Smith et al., 1985).

The next update of the AFGL compilation will be released in 1985. Major changes include the merging of the major gas and trace gas linelists into a single compilation, and expansion of the record length for each spectral line to accommodate additional parameters such as the temperature dependence exponent for the air-broadened halfwidth. Updates in the parameters for individual molecules are summarized below.

H_2O. Positions and intensities will be updated for lines in the 0.7- to 0.9-μm region, and for weak lines in the R-branches of the fundamental bands. Parameters for HDO will be updated in the 7-μm and pure rotation bands.

CO_2. Positions and intensities for all bands will be updated using the results of a global analysis currently in progress (R. Wattson and L. S. Rothman, private communication) which incorporates recent laboratory results

Table 3.1 Gases in AFGL Compilations

1. H_2O^*
2. CO_2^*
3. O_3^*
4. N_2O^*
5. CO^*
6. CH_4^*
7. O_2
8. NO^*
9. SO_2
10. NO_2^*
11. NH_3
12. HNO_3^*
13. OH
14. HF^*
15. $HC\ell^*$
16. HBr
17. HI
18. $C\ell O^*$
19. OCS
20. H_2CO
21. $HOC\ell$
22. N_2
23. HCN
24. $CH_3C\ell$
25. $H_2O_2^*$
26. C_2H_2 (acetylene)
27. C_2H_6 (ethane)
28. PH_3 (phosphine)

Other Gases of Interest

C_3H_8 (propane)
C_2H_4 (ethylene)
$CFC\ell_3$ (F-11)*
$CF_2C\ell_2$ (F-12)*
$CF_3C\ell$ (F-13)
$CHC\ell F_2$ (F-22)
$CHC\ell_2F$ (F-21)
$CC\ell_4$
CF_4
CF_3Br (F-13B)
$CH_3CC\ell_3$ (methyl chloroform)
$C_2F_3C\ell_3$ (F-113)
$C_2F_4C\ell_2$ (F-114)
$C_2F_5C\ell$ (F-115)
C_2F_6 (F-116 or perfluoroethane)

HO_2
HNO_2
HO_2NO_2 (peroxynitric acid)
NO_3
$N_2O_5^*$
$C\ell ONO_2$ (chlorine nitrate)*
CS_2
H_2S
H_2SO_4 (sulfuric acid)
SO_3
CF_2O (difluorophosgene)
$CFC\ell O$ (chlorofluorophosgene)
CH_2O_2 (formic acid)
CH_3OH (methanol)
CH_3CN (acetonitrile or methyl cyanide)

*indicates species to be measured by UARS from many sources, including AFGL, NASA Langley, JPL, Lab. d'Infrarouge in Orsay, University of Oulu, Finland, and Ohio State University. The most accurate results are expected for bands in the 2.7- to 15-μm regions, where nearly all the measurements were made.

$\underline{O_3}$. Air-broadened halfwidth values will be updated for all $^{16}O_3$ bands based on calculations by Gamache and Davies (1985) for the ν_1 and ν_3 fundamentals. Positions and intensities will also be updated for the pure rotation, ν_1, ν_3, and $\nu_1+\nu_2+\nu_3$ bands.

$\underline{N_2O}$. Intensities will be updated for vibration-rotation bands in the 900- to 2600-cm^{-1} region. Halfwidths for several bands will also be updated.

CO. Very accurate positions (± 0.25 Doppler width) and intensities (± 5 percent) from the work of Chackerian et al. (1983) have been adopted.

$\underline{CH_4}$. Parameters have been improved for the 7-μm, 5.8-μm, 3-μm, and 2.3-μm regions, mainly through the work of L. Brown (private communication).

NO. Halfwidths in the fundamental band will be updated.

$\underline{SO_2}$. Positions and intensities in the pure rotation bands and the 19-μm, 8.7-μm, and 7.3-μm regions will be updated using data from JPL and NBS.

$\underline{NO_2}$. Positions and intensities will be updated in the pure rotation bands and in the 13-μm, 6.2-μm, and 3.4-μm regions using the work of Perrin et al. (1984) and other recent results.

$\underline{NH_3}$. Parameters updated on the most recent GEISA compilation will be incorporated into the AFGL compilation also.

$\underline{HNO_3}$. Improved parameters in the 11.3-μm region from the work of Maki and Goldman (private communication) will be used to update the compilation.

OH. Pure rotation lines in the 84- to 200-cm^{-1} region will be adopted from the JPL microwave catalog (Poynter and Pickett, 1980).

HF. Calculated DF positions and intensities from R. Tipping (private communication) will be added. Halfwidths from Thompson et al. (1984) will be adopted.

HCℓ. Halfwidth results from J. Ballard (private communication) will be incorporated.

CℓO. Halfwidths from the microwave measurements of Pickett et al. (1981) will be adopted.

OCS. Positions and intensities will be updated for several bands in the 5- to 16-μm region.

$\underline{H_2CO}$. Pure rotation lines will be added from the JPL catalog.

HOCℓ. Pure rotation lines will be added from the JPL catalog.

HCN. Intensities and halfwidths in the 3-μm region will be updated using the results of Smith et al. (1984) and Varghese and Hanson (1984).

H_2O_2. Pure rotation lines will be added from the JPL catalog.

C_2H_2. Hot bands and isotopic bands in the 13.7-μm region will be added.

C_2H_6. Parameters may be updated in the 12-μm and 3.3-μm regions, if new results from Tennessee and Denver are received by January 31, 1985.

The 1984 version of the GEISA data bank contains parameters for nearly 325,000 spectral lines belonging to 37 different molecules. The GEISA compilation differs from the existing AFGL compilation in several major aspects.

1. There are no separate major-gas and trace-gas compilations.

2. In addition to molecules of terrestrial importance, molecules relevant to the study of other planetary atmospheres are included. These are C_2H_4, GeH_4, C_2N_2, C_4H_2, HC_3N, H_2S, HCOOH, and $^{13}C^{18}O_2$.

3. Isotopic variants whose symmetry is significantly different from the "normal" molecule (e.g., CH_3D) are considered to be separate molecular species.

4. For certain molecular species, such as CH_4, which are important for the atmospheres of the giant planets, the lower-limit cut-off for line intensities is different from that of AFGL.

5. Only data referenceable by published journal articles are included.

6. An additional parameter, the exponent for the temperature dependence of the air-broadened halfwidth, has been added. The exponent n is given by:

$$\gamma(T) = \gamma(T_0)(T_0/T)^n \qquad (3.1)$$

where γ is the broadening coefficient in cm^{-1}/atm, T is the actual temperature in degrees K and T_0 is the reference temperature (296 K). Based on measurements available in the literature, values of n have been added to the GEISA compilation for these 10 molecules: H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NH_3, CH_3D, and C_2H_2. The procedure for accessing this new parameter is described in an internal report by Chedin et al. (1985) at the Laboratoire de Meteorologie Dynamique. The status of GEISA in 1984 is described in a paper by Husson et al. (1985).

Calculated spectra based on parameters in the AFGL have been compared to laboratory spectra recorded on the Kitt Peak FTS by L. Brown and co-workers. These comparisons illustrate the need for additional laboratory measurements of "well-known" molecules such as CO_2, H_2O, and CH_4. In the 15-μm region there are numerous weak CO_2 bands for which line positions and intensities given in the compilation differ significantly from those observed in the laboratory spectra. For H_2O between 1000 and 4000 cm^{-1}, the agreement between observed and calculated spectra is reasonably good, except for weak lines in the ν_2 band. For CH_4 the comparisons show that in the 7-μm region, improvements are needed in parameters for the $^{12}CH_4$ hot bands and the ν_2 fundamental band of $^{13}CH_4$. Hot band and isotopic band parameters also need improvement in the 3-μm region. CH_4 parameters for the 3700- to 4100-cm^{-1} and 5000- to 5500-cm^{-1} regions are completely lacking in the compilation, although lines do appear in laboratory spectra of these regions. In the 1.6-μm region, the CH_4 $2\nu_3$ band intensity needs to be corrected.

A. Goldman has done extensive comparisons of calculated spectra with atmospheric spectra recorded from balloon and aircraft platforms. In the 860- to 900-cm^{-1} region, the new HNO_3 parameters to be included in the 1985 update of the AFGL compilation result in very good agreement between calculated and observed atmospheric spectra. However, in the 1260- to 1350-cm^{-1} region, the lack of good HNO_3 line parameters makes it very difficult to quantitatively analyze the $C\ell ONO_2$ absorption feature at 1292 cm^{-1} in atmospheric spectra. More accurate parameters for weak CH_4, N_2O, and CO_2 lines are also needed in this region. The $C\ell ONO_2$ Q-branches at 780 cm^{-1} and 805 cm^{-1} are very favorably located for atmospheric retrievals, provided that accurate parameters for the interfering ν_2 band of O_3 become available. The ν_6 Q-branch of formic acid (HCOOH) at 1105 cm^{-1} has been tentatively identified in spectra of the upper troposphere. However, the accuracy of quantitative analysis depends on improvements in line parameters for both HCOOH and interfering species, especially O_3. The spectral regions at 780 to 800 cm^{-1} and 2840 to 3100 cm^{-1} are favorable for spectroscopic measurements of atmospheric ethane (C_2H_6). Improved line parameters, especially intensities for ethane, are needed in both regions.

4. SUMMARY DISCUSSION AND RECOMMENDATIONS

Over the years that the AFGL and GEISA line parameter compilations have been in existence, various users have requested that additional information be included in the record for each spectral line. At the time when most computer users were constrained by 80-column card format, it was felt that additional data per line could not be included. Since most data transfer is now accomplished by magnetic tapes and disks, the 80-column restriction seems no longer relevant. Therefore, a major change in the AFGL compilation format has been proposed for the 1985 update, expanding the field beyond an 80-character width to accommodate additional data such as the halfwidth temperature dependence exponent (already included in GEISA), pressure-induced line shift, self-broadened halfwidth, transition probability, and uncertainty or reference codes for each parameter. The wider field would also allow additional decimal places so that line positions and lower state energies could be given with greater precision. This extra information cannot be added for every spectral line in the compilation before the release of the update in 1985, but the fields would be set aside for future entry of such information.

There seemed to be considerable support among the workshop participants for the proposed expansion in format. Most of the discussion centered on possible methods to "tag" the source of each parameter and indicate its accuracy, without making the compilation too cumbersome to use. Larry Rothman proposed that a simple reference number be listed for each parameter, with the references given in a separate table or report. Similar "table look-up" procedures could also be applied to streamline the representation of line assignments and isotope codes. It was suggested that the AFGL follow the example of GEISA and include only referenceable published data in its compilation. Some of the parameters in the present AFGL compilation are available only from unpublished reports or private communications. Fortunately, most of these are very old values and are gradually being replaced by more recent data published in the open literature.

In the final workshop session, there was some discussion of UARS timetables for including new spectroscopic parameters in data reduction algorithms. Many of the UARS data reduction algorithms are already under development, and all are expected to be in place before the 1989 launch date. It is desirable to have all the spectroscopic parameters at the required accuracy as soon as possible to allow algorithm testing with accurate simulated data. However, improved spectroscopic data could be incorporated at any time until the data reduction is finalized. There was also concern that the mechanisms for funding spectroscopic research in direct support of UARS should be made known to laboratory investigators. The UARS Spectroscopy Working Group plans to use its requirements document as a means of encouraging unsolicited research proposals to NASA from U.S. laboratories. While the excellent work at foreign laboratories is recognized to be of benefit to UARS goals, the direct funding of research at these labs presents many bureaucratic difficulties.

Recommendations for future spectroscopic research to meet UARS requirements, generated from the discussions of this workshop, are listed below.

General Recommendations

1. Accurate line parameters for the "major gases" (H_2O, CO_2, O_3, N_2O, CO, CH_4, and O_2) are needed in all spectral regions from 2.2 μm to the microwave, because of their interfering absorption. The most urgent needs are for line positions and intensities in weak bands (especially isotopic and hot bands), and for halfwidths and far-wing line shapes of strong lines.

2. Since information on the temperature dependence of halfwidths has been reported in the literature for only a small number of spectral lines for 10 atmospheric gases, measurements of air-broadened halfwidths and their temperature dependence from 190 K to 300 K are needed for all species of interest.

3. Measurements of self-broadened and N_2-broadened halfwidths and their temperature dependence over the range of temperatures to be encountered during instrument operation are needed for molecules to be measured using gas correlation or PMR cells ($HC\ell$, HF, NO, CH_4, CO_2, H_2O, N_2O, CO, NO_2).

4. An intercomparison of laboratory measurements of intensities and halfwidths for some "standard" set of pressure and pathlength conditions for a well-known gas (such as CO) might be useful for determining the absolute accuracy with which these quantities can be measured. The intercomparison would aid in understanding inherent differences among the various instruments and analysis techniques.

5. The existing line parameter compilations (AFGL or GEISA) serve as a useful repository for spectroscopic data. However, due to the limited personnel available to maintain these compilations, experimenters should submit their results on magnetic tape in the appropriate format to ensure more rapid updating of the compilations.

6. Laboratory spectroscopists should be informed about the mechanism for submitting proposals in response to UARS spectroscopic requirements. Methods for funding work at foreign labs with no formal UARS connection should be explored.

Specific Recommendations

H_2O. Positions and intensities are needed for weak lines in most spectral regions. Halfwidths, line shapes, and their temperature dependence are needed for all lines.

CO_2. Positions and intensities are needed for weak lines in most spectral regions, particularly at 2.7 μm. Halfwidths, line shapes, and their temperature dependence are needed for all lines.

O_3. Line positions and intensities are needed for isotopic and hot bands in the 10-μm region and for $^{16}O_3$ in the 13-μm and 3.3-μm regions.

CH_4. Positions and intensities are needed for weak lines, including isotopic and hot bands, in the 7.5-μm, 3.3-μm, and 2.5-μm regions. Self-broadened and air-broadened halfwidths and their temperature dependence are needed especially in the 7.5-μm and 3.3-μm regions.

O_2. Accurate measurements are needed for the collision-induced fundamental band over the temperature range from 190 to 300 K.

NO. Air-broadened and self-broadened halfwidths in the 1-0 band and their temperature dependence are needed.

NO_2. Line positions need to be corrected in the ν_2 band at 750 cm^{-1}.

HNO_3. The accuracy of calculated positions and intensities should be verified with additional measurements in the 12-μm, 7.5-μm, and 5.7-μm regions.

HF and HCℓ. Additional accurate measurements are needed of intensities; self-broadened, N_2-broadened, and air-broadened halfwidths; line shapes; and their temperature dependence in the 1-0 bands.

CℓO. Additional measurements of intensities in the 1-0 band are needed. Air-broadened halfwidths in this band are also desirable.

$CFC\ell_3$ and $CF_2C\ell_2$ (F-11 and F-12). More precise representations of these bands for inclusion in line-by-line calculations are needed.

N_2O_5. Precise measurements of band intensities are needed, particularly in the 7.5-μm region.

$C\ell ONO_2$. Measurements of intensities for the bands at 780 cm^{-1}, 805 cm^{-1}, and 1292 cm^{-1} are needed.

Other spectroscopic needs not of immediate importance to UARS, but relevant to other remote sensing efforts such as ATMOS, were also briefly discussed. These are listed below.

$\underline{NH_3}$. Positions in the ν_4 band and intensities in the ν_2, ν_4, and $2\nu_2$ bands should be improved.

$\underline{OH}$. Rotational line positions for wavenumbers higher than 300 cm^{-1} are needed.

$\underline{CH_3C\ell}$. Additional positions and intensities in the ν_1 band near 2967 cm^{-1} should be determined. Parameters for ν_2 and ν_5 bands near 1300 cm^{-1} are also desirable.

$\underline{C_2H_6}$. Parameters are needed in the 12-μm and 3.3-μm regions.

$\underline{HO_2\text{, HCOOH, and HOC}\ell}$. Additional measurements of positions and intensities are needed to verify the few existing values.

$\underline{HNO_2\text{, }HO_2NO_2\text{, }CC\ell_4\text{, and }CF_4}$. Precise band intensity measurements are needed.

Other "Freons" (F-22, F-113, etc.). Intensity measurements and band representations are needed.

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16. Abstract

This report summarizes the informal discussions which took place during the Spectroscopic Parameters Workshop held at NASA Langley Research Center, October 17-18, 1984. The objectives of the workshop included communication of spectroscopic data requirements for the planned Upper Atmosphere Research Satellite (UARS) mission, review of the status of currently available spectroscopic parameters, and recommendation of additional studies. These objectives were accomplished and resulted in a series of general and specific recommendations for laboratory spectroscopy research to meet the needs of UARS and other atmospheric remote sensing programs.

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