



THE 7TH HITRAN DATABASE CONFERENCE
12-14 JUNE 2002

HARVARD-SMITHSONIAN CENTER FOR ASTROPHYSICS
CAMBRIDGE MA
USA



THE WORLD ACCORDING TO **GOME**



THE 7TH BIENNIAL HITRAN DATABASE CONFERENCE

12-14 June 2002
Phillips Auditorium
Harvard-Smithsonian Center for Astrophysics
Cambridge MA

Wednesday, 12 June

8:30 Registration

9:00 WelcomeLaurence Rothman

9:10 A User's View of HITRANReinhard Beer

SESSION 1: DATABASE AND REMOTE-SENSING ISSUES

Chair: Kelly Chance

9:40 Summary of Workshop on Molecular Spectroscopy for Atmospheric Sensing
.....Kenneth W. Jucks

10:10 JavaHAWKS EmpowermentKuilian Tang

10:30 *Break*

11:00 ..A Critical Review of O₃ and NO₂ Cross-Sections in the UV-Visible
.....Johannes Orphal

11:30 The Synergism Between Laboratories and Databases Related to Atmospheric Spectroscopy
.....Prasad Varanasi

Noon *Lunch*

SESSION 2: DATABASE COMPILATION

Chair: John J. Hillman

2:00 Evolution and Construction of the 12-micrometer Ethylene Spectral Atlas
.....William E. Blass

2:30 Recent Advances in Ozone High-Resolution Studies
.....Alain Barbe

3:00 HITRAN Indices of Refraction and Cross-Section Data
.....Steven T. Massie

POSTER SESSION 1: DATABASE AND REMOTE-SENSING ISSUES

Chair: Thomas Kurosu

3:30 – 5:30

(continued)

Thursday, 13 June

SESSION 3: SPECTROSCOPIC PARAMETERS

Chair: Johannes Orphal

9:00 Line Intensity Measurements in $^{14}\text{N}_2^{16}\text{O}$ and Their Treatment Using the Effective Operator Approach. II. The 5200- to 6400- cm^{-1} Region

.....Jean Vander Auwera

9:30 New analysis of the $\nu_5+\nu_9-\nu_9$ hot band of HNO_3

.....Jean-Marie Flaud

10:00 Nitric Acid Absolute Band Intensities between 820 cm^{-1} and 3600 cm^{-1}

.....Charles Chackerian, Jr.

10:30 *Break*

11:00 Rotational Spectroscopy and Infrared Band Simulations of Nitric Acid and Chlorine Nitrate

.....Douglas T. Petkie

11:30 New Cross-Sections and Line Parameters from the RAL Molecular Spectroscopy Facility

.....David Newnham

Noon *Lunch*

SESSION 4: SPECTROSCOPIC PARAMETERS

Chair: William Parkinson

2:00 Weak Water-vapor Spectrum in the Near Infrared and Optical Region

.....Roman N. Tolchenov

[Late change to Program:

The presentation by Roman Tolchenov, has been replaced by

“First Analysis of Preliminary ICLAS-Time-Resolved FTS Spectra”Victor Dana]

2:30 Water, Water, Water and a bit of Ozone.....Michel Carleer

3:00 The Application of a Vacuum Ultraviolet Fourier Transform Spectrometer and Synchrotron Radiation Source to Measurements of NO Bands

.....Kouichi Yoshino

POSTER SESSION 2: NEW SPECTROSCOPIC DATA

Chair: Ken Jucks

3:30 – 5:00

6:00 – 9:00 **BANQUET**

8:30 Grand Tour of Astronomy Facility (weather permitting)

(continued)

Friday, 14 June

SESSION 5: LINESHAPE ISSUES

Chair: Jean-Marie Flaud

- 9:00 Infrared Laboratory Measurements of HCN Broadened by N₂ and Air
.....Curtis P. Rinsland
- 9:30 Vibrational Dependence of Broadening and Shift Parameters for Linear Molecules
.....Mary Ann H. Smith
- 10:00 Extrapolation of Experimental Line-Width Data to Higher Rotational Quantum Numbers in
the Case of Linear Molecules as Applicable to the Atmosphere
.....Chengbo Sun
- 10:30 *Break*
- 11:00 Rotational Lineshape Parameters of Atmospheric Trace Species
.....Brian J. Drouin
- 11:30 Effects of Line Mixing Upon Spectroscopic Line Parameters in the R Branch of the 1-0 Band
of CO.....D. Chris Benner
- 12:00 Spectroscopic Study for an Airborne Image Interferometer for the Analysis of Combustion
Products from Biomass Burning.....Donatella Guzzi

END OF MEETING

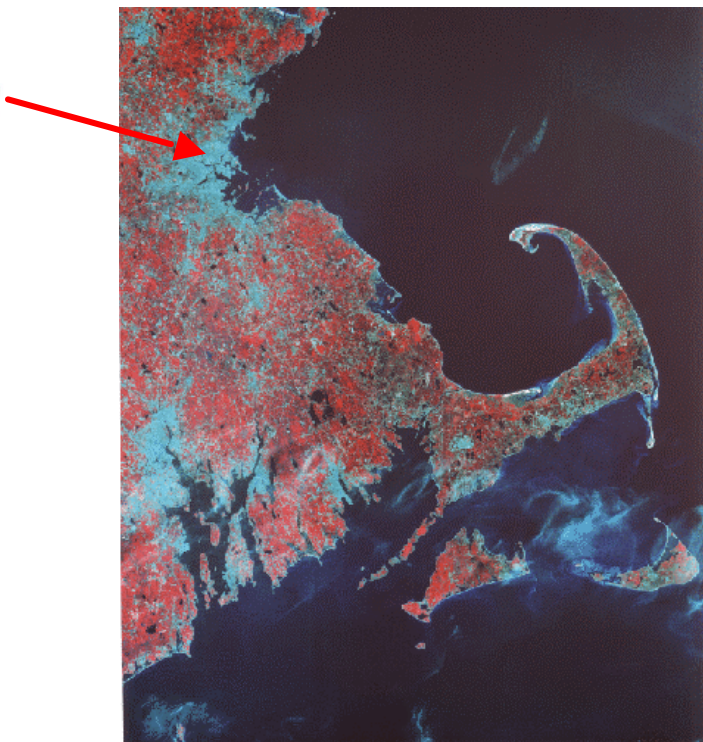


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A User's View of HITRAN

Reinhard Beer

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This talk will cover some of the issues that have arisen during a number of years of using HITRAN to analyze tropospheric infrared spectra from an airborne platform and to prepare for the forthcoming Tropospheric Emission Spectrometer (TES) to be launched in 2004 on the EOS (Earth Observing System) AURA spacecraft.

Summary of Workshop on Molecular Spectroscopy for Atmospheric Sensing

Kenneth W. Jucks

*Harvard-Smithsonian Center for Astrophysics
Optical and Infrared Astronomy Division, Cambridge MA 02138, USA*

A workshop, sponsored by the NASA Upper Atmosphere Research Program, was held in late October 2001 in San Diego whose purpose was to bring together researchers who use spectroscopic techniques to monitor the atmosphere with researchers who perform laboratory molecular spectroscopy with aims to prioritize the current spectroscopic needs of the atmospheric sensing community, communicate these needs to both the funding agencies and the spectroscopic community in general, and to communicate to the atmospheric sensing communities the current abilities of laboratory spectroscopy. The sessions were divided up into specific wavelength regions since individual atmospheric instruments tend to be restricted to one region. Each session consisted of overview talks that summarized the current atmospheric sensing techniques and atmospheric requirements and talks that summarized the current status of laboratory spectroscopy in each spectral region. These sessions were augmented by poster sessions that contained more detailed information of individual research efforts. These sessions were followed by discussions and breakout groups which made specific recommendations. I will summarize the conclusions from each wavelength region, as well as recommendations that were made for atmospheric spectroscopy databases in general.

JavaHAWKS Empowerment

Kuilian Tang^a, John Schroeder^a, Laurence S. Rothman^b

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North Andover MA, USA*

^b*Harvard-Smithsonian Center for Astrophysics
Atomic and Molecular Physics Division, Cambridge MA 02138, USA*

JavaHAWKS (HITRAN Atmospheric Workstation) is a software package to manipulate the HITRAN and associated molecular spectroscopic databases. It has been written in the Java programming language to make it platform independent. It allows the user to extract portions of data from line-by-line parameter files based on selection criteria, such as spectral range, molecules, isotopomers, bands, temperature, etc. The new edition of HITRAN has an expanded format for each line transition. The JavaHAWKS software works with both the existing 100-character per line format and the new 160-character line format.

Features of the software include: plotting of line-by-line and cross-section files; internet access of HITRAN and related databases; access to archival HITRAN documentation; and links to abstracts that are the sources for HITRAN parameters.

This presentation will include an interactive demonstration of the JavaHAWKS software.

The current effort has been funded by the NASA Earth Observing System (EOS), Grant NAG5-8420.

A Critical Review of O₃ and NO₂ Cross-Sections in the UV-Visible

Johannes Orphal^a and Joerg Callies^b

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F-91405 Orsay, FRANCE*

*^bEarth Observation Programmes Development Department
ESA/ESTEC, NL-2200 AG Noordwijk, The NETHERLANDS*

Atmospheric O₃ and NO₂ concentrations are currently measured using spectroscopic remote-sensing techniques in the ultraviolet and visible regions around 230-800 nm. One important source for uncertainties and/or systematic errors in the atmospheric concentrations determined is the choice of reference cross-sections from laboratory measurements. In the frame of a scientific study supported in 2001 by the European Space Agency ESA-ESTEC, Earth Sciences Division, the available laboratory cross-sections of O₃ and NO₂ at different temperatures and pressures have been compared, and some recommendations have been proposed.

The Synergism Between Laboratories and Databases Related to Atmospheric Spectroscopy

Prasad Varanasi

*State University of New York at Stony Brook
Institute for Terrestrial and Planetary Atmospheres
Stony Brook NY, USA*

In this talk the author presents data from his laboratory, emphasizes the need for data that are actually usable in atmospheric applications. The need to review, validate and revise what have become indispensable spectroscopic databases is advocated. The need for financial support from the agencies that benefit from the databases is voiced. Right now the entire burden of creating and maintaining the HITRAN and GEISA databases seems to be in the hands of just the two people who happen to be the custodians. Should anything happen to these two precious people or should they get tired of carrying this burden beyond 2004, possible successors should be named and trained. While the databases, far from being comprehensive or extensive, are in better shape now than they were a few years ago, the most important aspect, namely the temperature dependence of the spectral line parameters is very poorly archived due to the gross lack of accurate and extensive laboratory data. Every possible effort to remedy this deficiency should be addressed, discussed, debated and passed on to the funding agencies as a most pressing problem faced currently by the atmospheric spectroscopic community. Measurements made at room temperature, while valuable to the molecular spectroscopist from an academic point of view, are absolutely useless in atmospheric applications if the temperature dependence of the line parameters is not determined conclusively. This is a legacy that we cannot pass on to the next generation.

Evolution and Construction of the 12-micrometer Ethylene Spectral Atlas

William E. Blass^a and John J. Hillman^b

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Dept. of Physics and Astronomy, Knoxville TN, USA*

^b*NASA/Goddard Space Flight Center
Laboratory for Extraterrestrial Physics, Greenbelt MD, USA*

We tell the story behind the evolution and construction of the ethylene planetary modeler's atlas, the scientific publication of which is: ***10- μ m Ethylene: Spectroscopy, Intensities and a Planetary Atlas.***¹

1. W.E. Blass, J.J. Hillman, A. Fayt, S.J. Daunt, L.R. Senesac, A.C. Ewing, L.W. Jennings, J.S. Hager, S.L. Mahan, D.C. Reuter, and M. Sirota, *JQSRT* **71**, 47-60 (2001).

Recent Advances in Ozone High-Resolution Studies

Alain Barbe

Université de Reims-Champagne-Ardenne

Groupe de Spectrométrie Moléculaire et Atmosphérique CNRS, F-51687 Reims, FRANCE

The systematic study of the ozone molecule continues in the GSMA with the help of a high-resolution Fourier transform spectrometer, and the use of large product $p \times l$ (pressure \times pathlength). Many works have been published^{1,2,3} after the analysis of line positions and intensities. They were mainly concerned with relatively high energy levels $3000 < E < 6000 \text{ cm}^{-1}$. We recently extend these analyses to the lower energy levels (including the three fundamentals ν_2 , ν_1 , ν_3 , the first overtones $2\nu_2$, $2\nu_1$, $2\nu_3$ as well as the first combination bands $\nu_1 + \nu_2$, $\nu_2 + \nu_3$, $\nu_1 + \nu_3$). The observation of transitions assigned to very large values of J (up to 81 for ν_3) and K_a (up to 25 for ν_2) allows one to improve the sets of spectroscopic parameters. The agreement between observation and calculations is extremely satisfactory: the rms for 3500 transitions of the ν_3 band is $0.10 \times 10^{-3} \text{ cm}^{-1}$. Intensities are also derived, leading to new sets of transition-moment parameters and to good agreement between observations and calculations.

In addition, the $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ isotopomers have also been analysed in the whole spectral range between 900 and 5000 cm^{-1} , leading to the complete analysis of 13 rovibrational bands for $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ and 11 for $^{16}\text{O}^{18}\text{O}^{16}\text{O}$. All these new results are presented and are in due course to be incorporated into the S and MPO website^{4,5,6}: <http://ozone.univ-reims.fr>, <http://ozone.iao.ru>.

1. S.N. Mikhailenko, A. Barbe, V.I.G. Tyuterev, and A. Chichery, *Atmos.OceanicOpt.* **12**, n°9, (1999).
2. S.N. Mikhailenko, A. Barbe, J.J. Plateaux, and V.I.G. Tyuterev, *J.Mol.Spectrosc.* **196**, 93-101 (1999).
3. A. Chichery, A. Barbe, V.I.G. Tyuterev, and M.T. Bourgeois, *J.Mol.Spectrosc.* **206**, 1-26 (2001).
4. S.N. Mikhailenko, S.N. Babikov, V.I.G. Tyuterev, and A. Barbe, MODAS conference paper 05.1 Irkutsk (2001).
5. V.I. G. Tyuterev, A. Barbe, Yu. Babikov, and S.N. Mikhailenko, XVIIth colloquium on High resolution Molecular spectroscopy, paper F28 Nijmegen (2001)
6. Yu.L. Babikov, A. Barbe, V.F. Golovko, S.N. Mikhailenko, and V.I.G. Tyuterev, Internet collections for molecular spectroscopy, Russian Conference on digital Libraries, Petrozavodsk, September 2001.

HITRAN Indices of Refraction and Cross-Section Data

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Gas molecules, aerosol particles, and heavy molecules including the CFCs and HCFCs all contribute to the opacity of the Earth's atmosphere. The HITRAN database includes indices of refraction for various composition types, and absorption cross-sections for several gas species. The indices and cross-sections are reviewed and evaluated, and radiative-transfer applications of the spectroscopic data are discussed. Additional laboratory measurement needs are also addressed.

PW1. JavaHAWKS Empowerment

Kuilian Tang^a, John Schroeder^a, Laurence S. Rothman^b

^a*Ontar Corporation
North Andover MA, USA*

^b*Harvard-Smithsonian Center for Astrophysics
Atomic and Molecular Physics Division, Cambridge MA 02138, USA*

JavaHAWKS (HITRAN Atmospheric Workstation) is a software package to manipulate the HITRAN and associated molecular spectroscopic databases. It has been written in the Java programming language to make it platform independent. It allows the user to extract portions of data from line-by-line parameter files based on selection criteria, such as spectral range, molecules, isotopomers, bands, temperature, etc. The new edition of HITRAN has an expanded format for each line transition. The JavaHAWKS software works with both the existing 100-character per line format and the new 160-character line format.

Features of the software include: plotting of line-by-line and cross-section files; internet access of HITRAN and related databases; access to archival HITRAN documentation; and links to abstracts that are the sources for HITRAN parameters.

The current effort has been funded by the NASA Earth Observing System (EOS), Grant NAG5-8420.

PW2. Millenium HITRAN Compilation

Laurence S. Rothman^a, Kuilian Tang^b, John Schroeder^b

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Atomic and Molecular Physics Division, Cambridge MA 02138, USA*

*^bOntar Corporation
North Andover MA, USA*

The current edition of the HITRAN molecular absorption compilation has been made available on an anonymous ftp-site located at the Harvard-Smithsonian Center for Astrophysics (<ftp://cfa-ftp.Harvard.edu/pub/HITRAN>). The compilation consists of five main folders: (1) the traditional line-by-line parameter database, (2) aerosol indices of refraction, (3) UV cross-sections and line-by-line parameters, (4) IR cross-sections, and (5) software and documentation. There are also extensive tables of partition sums covering a wide temperature range for all the isotopomers in HITRAN, and a high-temperature analog of HITRAN called HITEMP.

Some updates or corrections have been posted since the official release of the archival data in the ftp-site. These improvements are given in the public HITRAN web-site (<http://cfa-www.Harvard.edu/HITRAN>) and will be incorporated into the next edition. Collaborations with many research teams throughout the world have enabled great improvements in providing more accurate parameters, extended spectral coverage, and documentation. Besides the line-by-line absorption parameters, significant progress has been made for pressure-temperature sets of absorption cross-sections as well as increased tables of aerosol properties. A new edition of the HITRAN compilation is planned for 2002.

The format of the line-by-line portion of the HITRAN compilation is being expanded to accommodate larger polyatomic molecules, information for non-local thermodynamic equilibrium (NLTE) atmospheric dynamics and astrophysics, and improved documentation. The improvements not only will provide increased capabilities for atmospheric transmission/radiance calculations and re-mote sensing, but will allow access and analytical tools for related molecular databases.

The current effort has been funded by the NASA Earth Observing System (EOS), Grant NAG5-8420; and the Atmospheric Radiation Measurement (ARM) program of the Environmental Sciences Division, Office of Biological and Environmental Research, US Department of Energy.

PW3. Database Development for Terahertz Astronomy

Kelly V. Chance^a, Laurence S. Rothman^a, Kenneth W. Jucks^b, Carl A. Gottlieb^c

^aAtomic and Molecular Physics Division

^bOptical and Infrared Astronomy Division

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The THz region is gaining increased interest to astronomy as measurements become more technically feasible, suitable ground based observing sites are being developed, and the SOFIA Airborne Observatory becomes operational in 2005. There is currently no adequate comprehensive database of molecular parameters to guide spectral line astronomy in the THz region. Discussed here is an outline of the form and content of a THz database that will be compiled with consultation of the radio astronomy community at the Center for Astrophysics. It is evident that in addition to accurate line frequencies, a useful compilation should include quantities such as the Einstein-A coefficients and frequency uncertainties on the one hand; and terrestrial line intensities (with their temperature dependence), isotopic composition, and air-broadening coefficients on the other. Work is now in progress to develop a preliminary spectroscopic database for the 1 to 2 THz region. The species that have been considered include both neutral and ionized atoms, diatomic hydrides, a few additional diatomic molecules such as CO and CN, approximately 10 triatomic molecules, and several tetratomic molecules.

PW4. Quantitative, Infrared Spectral Libraries for Gas Samples

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The National Institute of Standards and Technology (NIST) and the Pacific Northwest National Laboratory (PNNL) are independently creating quantitative, $\sim 0.10 \text{ cm}^{-1}$ resolution, infrared spectral libraries of atmospherically broadened vapor-phase compounds. The NIST library will consist of approximately 100 vapor-phase spectra of volatile hazardous air pollutants (HAPs) and suspected greenhouse gases. The PNNL library will consist of approximately 400 vapor-phase spectra associated with DOE's remediation mission.

A critical part of creating and validating any quantitative work involves independent verification based on inter-laboratory comparisons. The two laboratories use significantly different sample preparation and handling techniques. NIST uses gravimetric dilution and a continuous flowing sample while PNNL uses partial-pressure dilution and a static sample. Agreement is generally found to be within the statistical uncertainties ($k = 2, 2s$) of the Beer's law fit and less than 3 % of the total integrated band areas for the chemical samples used in this comparison. There does appear to be a small (~ 1.5 %) systematic difference between the PNNL and NIST data, however.

PW5. The Spectral and Molecular Properties of Ozone (S&MPO) Databank

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The S and MPO databank (Spectral and Molecular Properties of Ozone) has been created^{1,2,3} one year ago (2001) and has been installed on the web on two sites:

<http://ozone.univ-reims.fr>

<http://ozone.iao.ru>

Many data have been introduced, mainly for $^{16}\text{O}_3$: spectroscopic parameters, transition-moment parameters, observed spectra, statistics for the fit for transitions and intensities, mostly for high energy levels ($>4000\text{ cm}^{-1}$) which were not included into HITRAN⁴ or GEISA⁵ databanks.

Since this time, we have performed new fits on the main bands for $^{16}\text{O}_3$: ν_2 , ν_1 , ν_3 , $\nu_1 + \nu_2$, $\nu_2 + \nu_3$, $2\nu_3$, $\nu_1 + \nu_3$, $2\nu_1$, with observations of rotational quantum numbers much higher than those used to derive spectroscopic parameters, and new calculations.⁶ These new spectroscopic parameters statistics of fits calculations and comparisons with observed spectra are now included in S&MPO. In addition, many spectroscopic studies of isotopomers are also recently done or are in course. Most of these studies are incorporated into this bank, in particular $^{18}\text{O}_3$ and $^{16}\text{O}^{18}\text{O}^{16}\text{O}$.

We present here these new data.

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1. S.N. Mikhailenko, S.N. Babikov, Vl. G. Tyuterev, and A. Barbe, MODAS conference paper 05.1, Irkutsk (2001).
 2. Vl. G. Tyuterev, A. Barbe, Yu. Babikov, and S. Mikhailenko, XVIIth colloquium on High Resolution Molecular Spectroscopy, paper F28, Nijmegen (2001)
 3. Yu. L. Babikov, A. Barbe, V.F. Golovko, S.N. Mikhailenko, and Vl.G. Tyuterev, Internet collections for molecular spectroscopy, Russian Conference on digital Libraries, Petrozavodsk, September 2001.
 4. L.S. Rothman, et al, *JQSRT* **60**, 665-710 (1998).
 5. N. Jacquinet-Husson, et al, *JQSRT* **62**, 205-254 (1999).
 6. G. Wagner, M. Birk, F. Schreier, and J.M. Flaud, *J.G.R.*, accepted (2002).

PW6. Does the 12-micrometer Ethane Database Need a Tune-up?

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Ethane at 12 μm is very rich, exhibiting ν_9 , $\nu_9 + \nu_4 - \nu_4$, $\nu_9 + 2\nu_4 - 2\nu_4$, etc. In the early 1980s, there was a flurry of activity in the study and analysis of ν_9 by several international collaborations – some of us dubbed the activities “The Ethane Wars”, which by the way were friendly competitions. Since the days of the Ethane Wars, much additional work has been carried out and published. Nonetheless, problems are still popping up when and where least expected. We attempt to illuminate the situation and make some suggestions for future efforts.

**PW7. HITRAN Usage in the Integrated Information-Computational System
“Atmospheric Optics” and in the Web Portal on Environmental Sciences
“ATMOS”**

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The HITRAN Database is one of the key elements of the scientific site “Atmospheric Spectroscopy” (<http://spectra.iao.ru/>) which is a part of the recently developed Integrated Information-Computational System “Atmospheric Optics”. The system also comprises sites “Atmospheric Models” (<http://model.iao.ru/>), “Atmospheric Chemistry” (<http://atmos.iao.ru/>) and “Atmospheric Aerosols” (<http://aerosol.iao.ru/>). It is a multi-user system aimed to be used via the Internet. A standard browser supports the user-system interface. All computational tasks are performed at the server side and usage of significant user resources is not required to this end. Parallel computations supported by the computer cluster are employed in the computational block of the system, in particular for solving of nonlinear equation sets for atmospheric chemistry. The “Atmospheric Spectroscopy” (<http://spectra.iao.ru/>) site provides user with information on spectral line parameters of atmospheric gases to be used for atmospheric optic problem solving. It allows one to get intensities, absorption coefficients, and transmission and radiation spectra at given wavelengths for chosen gas mixtures and optical paths.

More wide usage of the HITRAN is planned within the currently developed Web Portal on Environmental Sciences “ATMOS” (INTAS Project 00-189). The bilingual (Russian and English) scientific web Portal is designed as an integrated set of distributed but coordinated topical web sites, combining classical multi-media information with research databases, models and analytical tools for on-line use, and visualisation. Each site consists of data, models and visualisation functions.

The basic thematic sites integrated into the proposed ATMOS site are: Atmospheric Chemistry, Spectroscopy and Aerosols with a structured presentation of measurements of aerosol optical characteristics, chemical properties and microphysics, and atmospheric chemistry process description. Also it should provide researchers with the basic spectroscopy information on molecular atmospheric species and the opportunity to calculate the radiation propagation in non-homogeneous atmospheres; Solar-Terrestrial Relationships: radiation, atmosphere and geomagnetism providing measurements of solar radiation spectra and considerations of solar influence on atmospheric characteristics; Atmospheric Radiation to be used for calculations of radiation fluxes in the atmosphere and study of aerosols, clouds and the minor gas constituent's effect on the radiation regime; Dynamics of Atmosphere dealing with climatically and environmentally oriented models of different levels starting from 3-D GCM to statistical models of the Atmosphere.

Air Quality Assessment and Management site will compile basic aspects of air pollution and environmental impact assessment and include interactive tutorials.

Within the system framework, HITRAN will be employed to determine absorption along the chosen paths, to calculate relevant photochemical reaction coefficients and to calculate radiation fluxes in atmosphere. Usage of the HITRAN in the both systems should give this Database additional vision and expand the number of its potential users.

**PW8. State-of-the-art Ab Initio Prediction
of Molecular Vibration-Rotation Spectra**

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We have developed and implemented a new method for solving the eigenvalue equation of the molecular rotation-vibration quantum Hamiltonian. The accuracy of the spectra predicted by this method will be demonstrated on methane. A comparison will be made with lines available in the HITRAN database.

PW9. Lineshape Model Analysis for Measurements in the Microwave Region**J.-M. Colmont, F. Rohart, Georges Wlodarczak**

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We present relaxation studies performed in the millimeter and submillimeter range on various molecules of atmospheric interest: NO, N₂O, HNO₃, CH₃Cl, CO. The collisional broadening coefficients with O₂ and N₂ were determined, and their temperature dependence analyzed in the range 235-350 K. Some complementary data were obtained on nitriles (HCN, HC₃N, CH₃CN) mostly dedicated to planetary atmospheres (Titan). In the case of symmetric tops (CH₃CN, CH₃Cl), the *K* dependence of the collisional broadening coefficient was also investigated.

Besides the goal of providing accurate spectroscopic parameters allowing for fine analysis of atmospheric spectra, most of the reported measurements have given a clear evidence of line narrowing processes, that is, of a failure of the Voigt profile. The experimental observations have allowed tackling studies on the physical origin of frequently reported line narrowings. Up to a recent time and from a purely numerical point of view, it was generally recognized that Galatry and Speed Dependent Voigt profiles lead to an equal quality in the fitting of experimental lineshapes. As a consequence, it was not possible to distinguish between the two possible origins of narrowing effects: velocity/speed changing collisions (Dicke or diffusion process) or speed dependence of relaxation rates.

From our observations on CO and N₂O in collision with various perturbing gases (N₂, O₂, CO₂, H₂, rare gases), it is observed that the optical diffusion parameter involved in the Galatry profile may have a strongly nonlinear pressure dependence, in agreement with similar observations reported on infrared HCN lines.¹ As a general conclusion, it seems possible to claim that, except for the case of very light collision partners (He and H₂), narrowing effects originate mainly from the speed dependence of relaxation rates that have to be modeled by a Speed Dependent Voigt profile.

1. J.-F. d'Eu, B. Lemoine, and F. Rohart, *J.Mol.Spectrosc.*, in press, 2002.

PW10. The Program Complex for Computation of Spectroscopic Characteristics of Atomic and Molecular Gases in UV, Visible, and IR Spectral Range for a Wide Range of Temperatures and Pressures

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The program complex for calculations of spectroscopic properties of gases in UV, visible and IR ranges consists of:

- the algorithms describing spectroscopic characteristics of the neutral and ionized atoms and molecules,
- the package of applied programs for calculation on personal computer,
- a set of banks of initial given physical, thermodynamic and spectroscopic constants and parameters.

Our program complex allows one to compute parameters of hyper thin structure in electronic-vibrational-rotational spectrums of diatomic molecules (O₂, N₂, N₂⁺, NO, CO, CN, OH, CH, AlO, SiO, HF, HCl) such as wave numbers, widths, Honl-London factors, intensities of vibronic lines etc.

The program complex permit to carry out mathematical modeling and calculations of optical characteristics of heated gases (more than twenty neutral and ionized atomic and molecular particles) in ranges:

- temperatures: 200 - 10000 K;
- pressure: 10⁻⁵ - 10 atm;
- wavelengths: 0.1—25.0 mkm or any spectral intervals inside this rang.

Input parameters of the program system are temperature (equilibrium or non-equilibrium), partial pressure of chosen components of gas mixture, spectral range and width of apparatus function.

Output dates of the program system are absorption coefficients, absorption cross-sections and emissivity of chosen components of gas mixture.

**PW11. CO₂ Q-band Line-Mixing Implementation in HARTCODE
using HITRAN2000**

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Line-mixing model implementations in atmospheric radiative-transfer codes are sometimes complex. The sensitivity of the line-mixing parameterization to the individual lines raises the problem of compatibility of the absorption databases and the line-mixing models. In this paper, the implementation of Hartmann's CO₂ Q-band line-mixing model into the High-resolution Atmospheric Radiative Transfer Code HARTCODE and the necessary modifications of the HITRAN2000 database are discussed.

**PW12. Updates of Spectroscopic Data used in the
ILAS Version 6 Data Retrieval Algorithm**

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The Improved Limb Atmospheric Spectrometer (ILAS) observed polar stratospheric minor constituents such as O₃, HNO₃, NO₂, N₂O, CH₄, and H₂O from October 1996 to June 1997. The ILAS Version 5.20 Level 2 data products have been newly opened to the public via the Internet. Afterwards, several advancements of the ILAS data retrieval algorithms have been investigated for the ILAS Version 6 data release. Some of them are updates of spectroscopic data, which are used in the theoretical spectral calculation. The effects of these updates will be shown in this presentation. In the Version 6 algorithm, target species will be changed and added. This situation will also be presented here.

PW13. Fitting NO₂ Cross-sections to OSIRIS Spectra**Chris E. Sioris***Harvard-Smithsonian Center for Astrophysics
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In the 435-449 nm spectral range, the differential spectral structure observed in the stratosphere by the limb viewing OSIRIS (Optical Spectrograph and Infrared Imager System) onboard the ODIN satellite is dominated by NO₂ electronic absorption. I compare spectral fits using cross-sections measured in the laboratory by Vandaele *et al*¹ and Bogumil *et al*² at various temperatures which are subsequently convolved and binned for OSIRIS.

1. A.C. Vandaele, C. Hermans, P.C. Simon, M. Carleer, R. Colin, S. Fally, M.F. Mérienne, A. Jenouvrier, and B. Coquart, "Measurements of the NO₂ absorption cross-section from 42000 cm⁻¹ to 10000 cm⁻¹ (238-1000 nm) at 220 K and 298 K," *JQSRT* **59**, 171-184 (1998).
2. K. Bogumil, J. Orphal, S. Voigt, H. Bovensmann, O.C. Fleischmann, M. Hartmann, T. Homann, P. Spietz, A. Vogel, and J.P. Burrows, "Reference spectra of atmospheric trace gases measured the SCIAMACHY PFM satellite spectrometer," *Proc.Europ.Sympos.Atmos.Meas.Space*, 443-447 (1999).

**PW14. Spectroscopic Study of Least Attenuating Paths
in the Horizontal Atmosphere**

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We are planning a series of practice runs with lasers and masers of different wavelengths to explore the attenuation at different wavelengths and atmospheric conditions. We will primarily focus on horizontal paths in the atmosphere. The theoretical part of the investigation should provide insight into the range of laser power and wavelengths needed in the experimental part. Least attenuating paths will be theoretically investigated with the HITRAN database. We have plans to correlate the theoretical results with changes in climatic conditions also in order to discover dynamics of the least attenuating paths.

**PW15. KCARTA : A Fast Pseudo Line-by-Line Radiative Transfer Code
with Scattering**

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kCARTA is a pseudo line-by-line code that is the EOS-AIRS Reference Forward Model. The optical depths are rapidly computed from compressed lookup tables of pre-computed atmospheric molecular absorption coefficients, and can be used for any realistic Earth atmospheric situation. The absorption coefficients have been computed using HITRAN, and include our latest estimates of line-mixing parameters for CO₂ P/R-branch line mixing. We are currently analyzing water-vapor data to improve the self and foreign continuum coefficients in the 1600-cm⁻¹ region. Radiative transfer for either uplooking or downlooking instruments at arbitrary heights, can be computed both for clear-sky or for cloudy-sky conditions. The scattering codes used include DISORT, RTSPEC and kTWOSTREAM.

PW16. Partition Functions for the HITRAN Database

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A synopsis of the methods used for calculating partition functions for the HITRAN database and the resulting data will be presented.

Line Intensity Measurements in $^{14}\text{N}_2^{16}\text{O}$ and Their Treatment Using the Effective Operator Approach. II. The 5200- to 6400- cm^{-1} Region

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This work continues a series of publications devoted to the application of the effective operators approach to the vibrational-rotational treatment of linear triatomic molecules, aiming at the analysis and prediction of infrared spectra of such molecules. In that frame, the present work aims at describing line intensities of cold and hot bands of $^{14}\text{N}_2^{16}\text{O}$ in its ground electronic state in the spectral range above 3600 cm^{-1} . In nitrous oxide, vibrational interacting levels group in polyads as a result of the relation $2\nu_1 \sim 4\nu_2 \sim \nu_3$ existing between the harmonic frequencies. The polyads are identified by the so-called polyad number $P = 2\nu_1 + \nu_2 + 4\nu_3$. Because of the very large spectral range and number of data, the treatment is first done on a polyad-by-polyad basis.

The absorption spectra of N_2O at room temperature have been recorded in Brussels over the whole range between 3600 and 11000 cm^{-1} using a Bruker IFS120HR Fourier transform spectrometer. The measurement and analysis of absolute line intensities in the region between 4300 and 5200 cm^{-1} , involving bands associated with transitions corresponding to $\text{DP} = 7, 8$ and 9 , has been done recently.¹

The present work is the continuation of that contribution. We are now measuring absolute line intensities for cold and hot bands associated with transitions corresponding to $\text{DP} = 10$ and 11 , observed in the range from 5200 to 6400 cm^{-1} . Using wavefunctions previously determined from a global fit of an effective Hamiltonian to about 18000 line positions,² parameters of a corresponding effective dipole moment are then fitted to these experimental intensities. Results will be presented and discussed.

1. L. Daumont, J. Vander Auwera, J.-L. Teffo, V.I. Perevalov, and S.A. Tashkun, *J.Mol.Spectrosc.* **208**, 281-291 (2001).
2. A. Camparque, G. Weirauch, S.A. Tashkun, V.I. Perevalov, and J.-L. Teffo, *J.Mol.Spectrosc.* **209**, 198-206 (2001).

New analysis of the $\nu_5+\nu_9-\nu_9$ hot band of HNO₃

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Nitric acid, which is an important NO_x atmospheric reservoir molecule, exhibits a strong absorption in the 11- μm spectral region. Since this region, which corresponds to an atmospheric window, is one of the most commonly used for the retrieval of HNO₃ in the atmosphere it is essential to have the best possible corresponding spectral parameters. Updates of these spectral line parameters were recently performed in the last versions of the atmospheric databases. They concern the line positions and intensities not only of the two interfering cold bands ν_5 and $2\nu_9$ but also of the $\nu_5+\nu_9-\nu_9$ hot band. This hot band exhibits indeed a sharp and strong Q branch at 885.425 cm⁻¹ which is clearly observable in atmospheric spectra and is used for the retrievals. However, in spite of these recent updates, it proved that the spectral parameters of the $\nu_5+\nu_9-\nu_9$ HNO₃ hot band are not accurate enough to reproduce accurately the observed atmospheric HNO₃ absorption in ATMOS spectra. A more accurate analysis of this hot band using new laboratory high resolution Fourier transform spectra has been performed. As a consequence, new and more precise line positions and line intensities were derived leading to a significant improvement in the simulation of atmospheric spectra. In parallel, improved calculations of the cold-band line positions are in progress and the corresponding results will be described.

Nitric Acid Absolute Band Intensities between 820 cm⁻¹ and 3600 cm⁻¹**Charles Chackerian, Jr.^a, Steven W. Sharpe^b, Thomas Blake^b, Robert L. Sams^b**

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The spectral absorbance of nitric acid, obtained with 0.1 cm⁻¹ resolution and under nitrogen broadening conditions, was determined for a number of nitric acid bands in the 820-3600 cm⁻¹ frequency range. Intensity measurements done at 278 K, 290 K, and 323 K allow hot-band lower-state energies to be determined. Where there is overlap, we have excellent agreement with the integrated band intensities measured by Giver et al.¹

1. L. Giver et al, *J.Opt.Soc.Am.* **B1**, 715-722 (1984).

Rotational Spectroscopy and Infrared Band Simulations of Nitric Acid and Chlorine Nitrate

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Recent results of millimeter and submillimeter wave rotational spectroscopy of the $\nu_5/2\nu_9$ states of nitric acid¹ have been used to simulate the complex structure of the $2\nu_9 - \nu_9$ and $\nu_5 - \nu_9$ hot bands near 22 μm . The comparison data were obtained with a high resolution Bruker FTIR at various pressures and a temperature of 297 K. The combination of the quality and resolution of the infrared data and the complexity of the spectra of these interacting states represents a stringent test for the simulation. It is shown that the agreement is very good and that this approach is generally advantageous.

Additionally, an overview of the on-going studies of the millimeter and submillimeter wave rotational spectrum of several vibrational states in nitric acid and chlorine nitrate will be presented. With the successful synthesis of the 22- μm band of nitric acid, our attention is turning toward other states of atmospheric interest. Several of these high-resolution rotational studies should provide accurate and useful infrared simulations to the remote sensing community. Of particular interest is chlorine nitrate since the infrared spectrum is only partially resolved in the Doppler limit.

1. D.T. Petkie, T.M. Goyette, P. Helminger, H.M. Pickett, and F.C. De Lucia, *J.Mol.Spectrosc.* **208**, 121-135 (2001).

New Cross-Sections and Line Parameters from the RAL Molecular Spectroscopy Facility

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New temperature-dependent cross-sections and line parameters for a range of atmospheric species have been determined by a number of UK research groups from quantitative, high-resolution laboratory spectra recorded using the Bruker IFS 120HR Fourier transform spectrometer and variable path-length gas cells at the RAL Molecular Spectroscopy Facility (www.msf.rl.ac.uk).

Mid-infrared absorption cross-sections of acetonitrile, benzene, 1,3-butadiene, acetone, and ‘super-greenhouse’ gas trifluoromethyl sulphur pentafluoride (SF_5CF_3) will be reported together with a summary of the laboratory measurement techniques and error budget considerations. In the near-infrared (1-2 μm) region, cross-sections of O_2 , O_2N_2 , O_2Ar , acetaldehyde, formaldehyde, methanol, acetone, and isotopic CO_2 have recently been measured and, for water vapour, scaling factors determined from high-resolution (0.005 cm^{-1}) spectra to correct HITRAN2000 line intensities. In the $700\text{-}1300\text{ cm}^{-1}$ ($14.3\text{-}7.7\ \mu\text{m}$) region, water-vapour line parameters have been measured from pure and air-broadened water vapour spectra recorded at 243 and 296 K and with 32 to 512 metre optical paths. Validation of new near-IR/visible water-vapour databases (ESA-WVR and HITRAN2000) against ground-based atmospheric transmittance observations made using a high-resolution Bomem DA3.002 interferometer and automatic solar tracker at RAL will be described.

As well as reporting these new experimental results, recommendations for further improvement to the spectroscopic databases for satellite remote sensing, pollution monitoring/control, and climate applications will be made.

Weak Water-vapor Spectrum in the Near Infrared and Optical Region

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Progress is reported on assigning long path length Fourier Transform Spectra of water vapor including (a) H₂¹⁶O spectra reported by Schermaul et al.¹ and (b) isotopically enhanced spectra due to Chevillard et al.² At the same time, new potential energy and dipole surfaces are being developed which will give much more reliable predictions of both frequencies and intensities of water-vapor lines in this region.

1. R. Schermaul, R.C.M. Learner, A.A.D. Canas, J.W. Brault, O.L. Polyansky, D. Belmiloud, N.F. Zobov, and J. Tennyson, "Weak Line Water Vapor Spectra in the Region 13200-15 000 cm⁻¹," *J.Molec.Spectrosc.* (2002).
2. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, *Can.J.Phys.* **63**, 1112-1127 (1985).

Water, Water, Water and a bit of Ozone

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The FTS absorption spectrum of H₂O in the 13000 to 25000 cm⁻¹ spectral region has been investigated at high resolution (0.03 and 0.06 cm⁻¹) and at room temperature, using an absorption path of 600 meters easily attainable in the 50-meter base length of the GSMA (Reims, France) multiple pass absorption cell. Measurements have been performed under various pressure conditions (pure H₂O, H₂O mixed with various pressures of N₂ or dry air). From these measurements, new values for the line parameters (position, intensity, pressure broadening and shift) have been deduced. Due to the very long absorption path, many new weak lines have been observed and measured for the first time, leading to an almost doubling of the known lines in this spectral region. The linelist resulting from this work is available in HITRAN format at <http://www.ulb.ac.be/cpm/datafiles.html>.

Using the same experimental set up, low-resolution spectra of pure water in the 2500 to 22500 cm⁻¹ spectral region have also been recorded. From these low-resolution spectra, a water absorption continuum can be extracted. It is shown that it most probably arises from two distinct effects: (1) A hydration of the surface of the White-type mirrors inside the cell, showing saturation at about 2 hPa of water pressure; (2) The presence inside the cell of tiny (~ 0.8 microns) droplets at all pressures of water, even at pressures as low as 2 hPa.

The addition of dry air to the water in the cell does not change the shape or the amplitude of the continuum. In addition, after careful elimination of the water lines by division by a synthetic spectrum calculated using the line parameters retrieved from the high resolution spectra, very weak absorption bands superposed to the continuum appear. They are tentatively attributed to light absorption by dimers and/or the far-wings of the water lines.

New measurements on O₃, NO₂ and H₂CO have been performed using two FTS's working in parallel. At the exit window of the absorption cell, the beam of light is divided in two by a beamsplitter and sent to the two spectrometers, both recording spectra at the same time, one in the UV-Vis and the other in the IR. The idea is either to use the IR spectrum to enable the precise measurement of the pressure of the molecule scrutinized (this is particularly important in the case of gas mixtures or the formation of polymers), or to confirm the relative values of the cross-sections in the UV-Vis versus the cross-sections in the IR. These spectra are still under analysis and preliminary results are shown for ozone.

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The Application of a Vacuum Ultraviolet Fourier Transform Spectrometer and Synchrotron Radiation Source to Measurements of NO Bands

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The Imperial College VUV-FT spectrometer has been equipped with optically contacted, beam splitters made from single crystals of MgF₂ and the short wavelength performance has been demonstrated down to ~139 nm. To make ultrahigh resolution VUV photoabsorption cross-section measurements with the VUV-FTS, requires a pure continuum source below 190 nm and the best choice is synchrotron radiation from a storage ring facility. Moreover, a suitable zero-dispersion predisperser is available on beam line 12-B of the synchrotron radiation source at the Photon Factory. We therefore moved the IC VUV FT spectrometer from Imperial College, London to the Photon Factory, Japan to exploit the bandwidth-limited synchrotron radiation as a background source for FT absorption spectroscopy.

The VUV-FT spectra of all NO bands in the wavelength region 195-160 nm have been recorded with an instrumental resolution of 0.06 cm⁻¹ (about a half of the Doppler widths). Accurate line positions and cross-sections of the β(11,0) and ε(0,0) bands have been determined. The term values of the D(0) and B(11) levels will be presented. Absolute band oscillator strengths of the both bands have been obtained from the integration of cross-sections of individual line.

This work is partly supported by NSF Division of Atmospheric Sciences grant ATM-94-22854 to Harvard College Observatory, and by NASA Upper Atmospheric Research Program under Grant No. NAG5-484 to the Smithsonian Astrophysical Observatory. The FTS measurements at the Photon Factory were made with the approval of the Photon Factory Advisory Committee (94G367).

PT1. Line Shape and Intensity Studies of Near Infrared Transitions of Oxygen and Acetylene by Diode Laser Spectroscopy

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A high-resolution near infrared diode laser spectrometer has been used for the measurement of line shape of ro-vibrational transitions of atmospheric molecules in the 700-950 nm region. The phase-sensitive detected spectra recorded with 2f frequency modulation show second derivative line shape with enhanced sensitivity. The short time ripples of the laser frequency allow a resolution of 0.003 cm^{-1} . The measurements have been carried out for the oxygen atmospheric A-band and acetylene overtone-combination band in the 760 and 780 nm regions respectively. The observed line profiles are digitally recorded and least-squares fitted by using Voigt and Galatry soft-collision model line shape functions. The analysis yields highly accurate values of pressure broadening, collision narrowing and line strength parameters. The results of measurements for self-broadening and foreign gas broadening in the presence of nitrogen, oxygen, helium and air will be reported. Because of the ambient temperature conditions and the glass optics used, the spectrometer can be useful for atmospheric monitoring.

PT2. Collision-Induced-Absorption in O₂/CO₂ Mixtures**Yuri I. Baranov^a, Walter J. Lafferty^a, Gerald T. Fraser^a, Andre A. Vigasin^b**

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The mid-infrared Collision-Induced-Absorption (CIA) of CO₂/O₂ mixtures has been investigated at 0.5 cm⁻¹ for sample temperatures between 206 K and 293 K and an optical path length of 84 meters. As shown previously¹, the spectrum of pure CO₂ even at a relatively low sample pressure of one atmosphere exhibits distinct bound dimer spectra with A-type and B-type Q-branch transitions near the centers of the CO₂ bands at 1284.6 and 1387.9 cm⁻¹. Featureless CIA spectra are also observed under the bound dimer spectra.

The CIA induced spectra in the vicinity of the O₂ fundamental band near 1556 cm⁻¹ have also been studied.² The spectra consist of broad P-, Q-, and R-branches with small ripple structure, which is most distinctive on the R-side of the band. The O₂ band strength increases dramatically with CO₂ pressure. Increasing CO₂ pressure also significantly modifies the profile of the pure O₂ band. In particular, new band structures appear at the band center, which are attributed to A-type and B-type Q-branches of an O₂—CO₂ asymmetric rotor complex, having infrared transition moments along both the *a* and *b* inertial axes.

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PT3. Measurements of Photoabsorption Cross Sections and their Temperature Dependence for CO₂ in the 170nm to 200nm Region

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All the photochemical models for the predominately CO₂ Martian atmosphere are very sensitive to the amount of CO₂ and to the values and spectral details of the absorption cross sections of CO₂ in the region 170 nm-200 nm. Earlier we had measured and published absolute cross sections of CO₂ in the region 118.0 nm-175.5 nm at 295K and 195K.

We have recently extended these measurements from 170 nm to 200 nm at 300K and 195K. The new measurements have been carried out at high resolution with our 6.65-m normal incidence, photoelectric spectrometer. To measure the weak photoabsorption of the CO₂ bands in the wavelength region 170 nm to 200 nm, we required a high column density of the gas. We obtained this by using a multi pass technique, a White cell. The White cell was designed to have a distance of 1.50 m between two main mirrors, and was set for four, double passes making a path length of 12.0 m. CO₂ gas was frozen in a stainless-steel cylinder immersed in liquid nitrogen, and the frozen product (dry ice) was pumped by the diffusion pump for purification. The CO₂ was warmed up slowly and kept in the cylinder at high pressure. The CO₂ pressure used in the White cell was varied from 1 to 1000 Torr depending on the wavelength region, and was measured with a capacitance manometer (MKS Baratron, 10 Torr and 1000 Torr). We divided the spectral region into twenty sections of about 1.5-nm extent. At each scan range, another scan was obtained from the emission spectrum of the fourth positive bands of CO for wavelength calibration.

We acknowledge funding from NASA, grant NAG5-7859 to Harvard College Observatory.

PT4. Line Strengths and Half-widths of the N₂O Bands in the 2.0- to 2.8- μ m Region at Room Temperature

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There are several combination and overtone bands of N₂O in the 2.0- to 2.8- μ m region. The line positions and strengths of these bands have not been revised from the initial version of the AFCRL line parameters compilation to the latest HITRAN2K database. In order to validate the line strengths and the half-widths of HITRAN, the high-resolution spectra of N₂O in the near infrared region were obtained at room temperature. All of the spectra were measured with a high-resolution Fourier transform spectrometer Bruker IFS 120HR. Since the range of the band strengths of the N₂O bands in the 2.0- to 2.8- μ m region is quite large, we used the absorption cells with the path lengths of 8.75, 20.0, 67.1, and 100.0 cm. A nonlinear least-squares fitting technique was used to determine the line strengths as well as the self-, N₂-, and O₂-broadened half-widths. The squared transition dipole moments and Herman-Wallis factors were also determined using the weighted least-squares method. Differences between the measured line strengths and those of HITRAN were found for almost all the absorption bands.

Self- and air-broadened half-widths determined from the R-branch lines in the 2v₃ band located around 2.3 μ m agreed quite well with those of HITRAN and the results of recent high-resolution experiments. A very weak absorption band, which has not been compiled in HITRAN, was found in the spectral region from 4940 to 4880 cm⁻¹. On the contrary, the lines around 4336 cm⁻¹ that have been compiled in the HITRAN database do not appear in the measured spectra. For the v₁+4v₂ band centered at 3621 cm⁻¹, all lines of the R- and P-branches are compiled in HITRAN92, whereas all R-branch lines and P1-P24 lines are not compiled in the HITRAN96,2K databases.

PT5. Infrared Spectrum of Water Vapor as Applicable to the Atmosphere

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High-resolution measurements of the absolute intensities, self- and air-broadened half-widths, self- and air-induced line shifts, and the variation of these parameters with temperature are presented for the infrared lines of water vapor in the 600-2100, the 3000-4050, 7000-7450, and 8300-8800 cm^{-1} regions. The measurements were performed using a high-resolution Bruker IFS-120 HR Fourier-transform spectrometer and cryogenically cooled absorption cells. A multi-spectral-line-fitting algorithm developed in our laboratory was used to determine the line parameters from measured transmittance spectra. Our new data are compared with the entries in the HITRAN database¹ and the numerous data reported by Toth.² The dissertation of Remedios³ has been the only previously reported, but unpublished, experimental source for the temperature-dependence of the air-broadened line widths in this region, and the results from that source were entered into the HITRAN database. The values of the parameter n , which symbolizes the temperature-dependence of the line width, from the present work are compared with the 63 entries in the HITRAN database. Very large differences, which prove to be significant in atmospheric applications, have been identified.

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**PT6. ICLAS - Time Resolved FTS
Intensity Measurements by Multispectrum Fitting Approach.
First tests on H₂O With Absorption Paths up to 130 km**

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Time-resolved spectra are recorded around 9600 cm⁻¹ with the high-resolution time-resolved step-scan interferometer of LPPM¹ from an intracavity laser set-up based on a vertical-cavity surface-emitting semiconductor laser located in the open air of the laboratory. Spectral and time resolutions are respectively equal to 0.18 cm⁻¹ and 3.2 μs. H₂¹⁶O lines are observed in more than one hundred time-component spectra, simultaneously recorded with absorption path lengths varying in arithmetic progression from 20 up to about 130 km.

In order to test their consistency, and their ability to provide absolute line parameters, the recorded data have been processed using a multispectrum fitting program.² This procedure is an efficient tool to control, in this type of experiment, the equivalent absorption paths L_{eq} that are the only varying experimental parameter. In particular, the origin of the generation time and the saturation of L_{eq} with generation time must be well defined before retrieving accurate intensity parameters.

Examples of simultaneous adjustments of spectra covering the equivalent lengths range 20-130 km are presented. Even with data not initially recorded for lineshape analysis, the modelling of the spectra and of the line profiles are satisfactory. Significant relative line positions and intensities are obtained for H₂O lines, some of them being already present in HITRAN. These results demonstrate that time-resolved Fourier transform spectroscopy coupled with an intracavity laser absorption experiment provide, thanks to the multispectrum procedure, a very sensitive quantitative approach for the accurate determination of line parameters.

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**PT7. Progress in the Knowledge of C₂H₂ in the IR:
Update of the HITRAN Database**

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The acetylene molecule is important for atmospheric, planetary, and astrophysics applications. In order to improve the knowledge of C₂H₂, systematic measurements of line parameters have been performed. Two main spectral regions have been studied in this work. First, in the 13.6-**mm** region, line intensities were revisited for the ν_5 band and determined for some hot bands, allowing the updating of HITRAN. Second, in the 5-**mm** region, numerous line parameters, including positions, intensities, self-broadening coefficients, and self-shifting coefficients of lines belonging to 18 bands were measured. As HITRAN did not contain information in this region, a line list was created.

Intensities were also measured for some new lines in the 4.5-**mm** region, and a good agreement was observed between previous measurements, already present in HITRAN. Concerning the 3-**mm** region where two cold bands were already analysed in positions and intensities, but where the intensities of numerous hot lines are missing in HITRAN, a study is in progress, and preliminary results will be presented.

**PT8. Pure- and air-broadened Absorption Cross-Sections
for the Infrared Bands of Acetone**

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Infrared absorption cross-sections for acetone have been measured using a Fourier transform infrared spectrometer, over the region from 600 to 1800 cm^{-1} , with a spectral resolution of 0.03 cm^{-1} . Measurements were recorded at 6 different temperatures between 297K and 223K, and at a number of different pressures, both for the pure gas and the gas broadened with air. In addition to the broad continuum of the band, structure has been observed in the pure spectrum of the 1215 cm^{-1} band. The structure gradually reduces as the total pressure is increased but remains apparent at pressures of 150 torr. The cross-section data will be presented together with comparisons of integrated band strengths to previous work. The uncertainties in the cross-sections have also been estimated.

**PT9. Positions and Intensities for the ν_8 and ν_3
Vibrational Systems of CH₃OH**

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Line positions and intensities for the ν_8 and ν_3 bands of methanol are needed by various user communities, but this information is currently unavailable in the HITRAN database. The 10- μm methanol feature together with O₃ and NH₃ was observed in several California forest fires by NASA overflights a few year ago and recently once again in Australia fires. The 3- μm feature has been seen in numerous comets. The present work is aimed at producing a line list to be included in the HITRAN database. As a first step, line positions and intensities for ν_8 and ν_3 are modeled using a non-interacting band model. The current prediction abilities for unperturbed line positions are 0.02 cm^{-1} and 0.04 cm^{-1} for ν_8 and ν_3 , respectively, and the intensity accuracy is 8 for ν_8 .

Part of the research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with The National Aeronautics and Space Administration.

PT10. First High-resolution Analysis of the Six Fundamental Bands $\nu_1 - \nu_6$ of COF^{35}Cl in the 340-2000 cm^{-1} Region

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Concern about the implication of chlorofluorocarbons (CFCs) in atmospheric ozone depletion has led to numerous measurements of the concentrations of halogen-containing compounds in the stratosphere. Of the various possible oxidation products of CFC's in the stratosphere, carbonyl chlorofluoride (COFCl) may receive attention. COFCl is indeed formed by the photolysis and oxidation of freon11 (CFCl_3). High-resolution atmospheric infrared spectra are potential means of monitoring COFCl. However, there is only little information on the spectroscopy of this molecule in the literature. We have therefore recorded spectra of pure ^{35}Cl enriched and natural samples of COFCl at $\geq 3 \text{ 0.002 cm}^{-1}$ resolution with the BRUKER Fourier transform spectrometer at the University of Wuppertal. We present here the first high resolution analysis of the six fundamentals: ν_1 (CO stretching mode), ν_2 (C-F stretching mode), ν_3 (C-Cl stretching mode), ν_4 (CFCl bending mode), ν_5 (CFCl rocking mode), and ν_6 (out-of-plane bending mode) bands located at 1875.8256, 1095.0646, 764.3876, 501.5941, 408.8099 and 666.5862 cm^{-1} respectively for the COF^{35}Cl isotopic species of carbonyl chlorofluoride. The ν_3 , ν_4 , ν_5 and ν_6 bands which are mainly of A-type, B-type, B-type and of C-type, respectively, appear as unperturbed. On the other hand, both the ν_1 and ν_2 bands have a hybrid character (with both A- and B-type transitions), and the analysis of these two bands was complicated by numerous resonances. The excellent results obtained during the analysis should allow an unambiguous detection of COFCl in the lower stratosphere in either the 5.3-, 9.1-, or 13- μm region.

PT11. Trans Formic Acid Studied using Fourier Transform Infrared Spectra and Submillimeter Wave Measurements

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New high-resolution Fourier transform absorption spectra of formic acid were recorded at Brussels in the 570 to 800-cm⁻¹ spectral range. Starting from the results of previous studies a new and more extended analysis of the ν_7 and ν_9 bands of formic acid located at 626.166 and 640.725 cm⁻¹ respectively has been performed. In this way, more than 11000 lines were assigned, leading to the identification of 7¹ and 9¹ energy levels up to $J = 61$ and $K_a = 22$. In addition, the rotational spectrum of formic acid in the 7¹ and 9¹ excited vibrational states has been investigated in the millimeter and submillimeter spectral regions. The observed infrared energy levels and microwave transitions were satisfactorily reproduced using a theoretical model which takes into account the very strong A- and B-type Coriolis interactions linking the energy levels of the 7¹ and 9¹ vibrational states: more than 85 % of the infrared energy levels are reproduced to within 0.001 cm⁻¹, indicating clearly the quality of the model.

New results on the ν_6 and ν_8 bands will also be presented.

**PT12. Rotational Spectroscopy of van der Waals Complexes
of Environmental Interest: Difluoromethane and Dimethyl Ether**

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Both difluoromethane (CH_2F_2 DFM) and dimethyl ether ($(\text{CH}_3)_2\text{O}$ DME) are alternative compounds and massive uses are expected. DFM is a non-ozone depleting gas and a replacement for CFCs. Now R-410A (DFM 50%, CF_3CHF_2 50%) and R-407C (DFM 23%, CF_3CHF_2 25%, $\text{CF}_3\text{CH}_2\text{F}$ 52%) have been used for a commercial refrigerator. On the other hand, DME is an attractive ultraclean alternative fuel for diesel because it has a high cetane number of 60, a low boiling point of -25°C and high oxygen content of 35% by weight. Therefore, it is expected to be the replacement fuel for ordinary petroleum. Before their massive uses, the chemical and physical properties of these compounds should be thoroughly investigated so as to be able to access their effects on earth environments in advance.

We report Fourier transform microwave spectra of the $\text{CH}_2\text{F}_2\text{-CF}_2=\text{CH}_2$ and $\text{CH}_2\text{F}_2\text{-CF}_2=\text{CHF}$ complexes and the $(\text{CH}_3)_2\text{O}$ dimer, $(\text{CH}_3)_2\text{O-Ar}$, $(\text{CH}_3)_2\text{O-CF}_2=\text{CH}_2$ and $(\text{CH}_3)_2\text{O-CF}_2=\text{CHF}$ complexes. Precise rotational transition frequencies, rotational and centrifugal distortion constants, and structural parameters will be presented. These complexes, except for $(\text{CH}_3)_2\text{O-Ar}$, were found to be bound with three hydrogen bonds of which one was stronger and the other two were relatively weaker.

These data on the DFM and DME complexes should be useful for the study of intermolecular interactions, structures, and the behaviors in the atmosphere.

PT13. Laboratory Measurements of Optical Properties of PSC Particles**Robert A. McPheat^a, David A. Newnham^a, R.G. Grainger^b, John J. Remedios^c**

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Various types of known and potential PSC particles (including nitric acid hydrates, supercooled ternary solution (STS), and sulphate aerosols) have been studied using an aerosol generation system and 75 dm³-volume, variable temperature spectroscopic cell. Broadband infrared extinction spectra of the PSC particles were recorded by measuring optical transmittance through the cell using a high-resolution Fourier transform spectrometer. Simultaneous measurements of the near-IR and visible scattering by the particles were made using sensitive CCD spectrometers. Spectra will be reduced to sets of quantitative extinction together with temperature and pressure values, and estimates of their uncertainties. IR and visible refractive indices will be derived by fitting the extinction spectra, PSC chemical composition, and temperature data using computer programs based on Mie theory.

PT14. Spectral Line Parameters for the $^{12}\text{CO}_2$ and $^{13}\text{CO}_2$ Laser Bands

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High-resolution experimental determination of line intensities, self-broadening and self-shift coefficients of the two $^{12}\text{CO}_2$ laser bands ($\nu_3 - \nu_1$ and $\nu_3 - 2\nu_2^0$) centered near 960.9 and 1063.7 cm^{-1} , respectively, are made from analysis of 30 room-temperature, long-path laboratory absorption spectra recorded at 0.0053 cm^{-1} resolution with the McMath-Pierce Fourier transform spectrometer at the National Solar Observatory on Kitt Peak. The measured line intensities were further analyzed to derive the vibrational band intensities and Herman-Wallis coefficients. Measurements are also provided for air- and N_2 -broadening and pressure shift coefficients for the two corresponding $^{13}\text{CO}_2$ laser bands (located at 913.4 and 1017.6 cm^{-1} , respectively). We used a multispectrum nonlinear least-squares fitting technique to analyze the data. By combining the spectra of $^{12}\text{CO}_2$ and $^{13}\text{CO}_2$ in the same fit, we are able to obtain a consistent set of line parameters for both molecules. The results obtained for the $^{12}\text{CO}_2$ and $^{13}\text{CO}_2$ laser bands are compared with each other, with values in the HITRAN database, and with values reported in the literature for CO_2 bands. Comparisons revealed no significant differences in the broadening or shift coefficients between the two laser bands. The coefficients determined for the two isotopomers agreed closely.

**PT15. Application of Tunable Diode Laser Absorption Spectroscopy
using the 1740-cm⁻¹ Band to Measure Formaldehyde**

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The infrared absorption line strengths of formaldehyde (H₂CO) from selected absorption features (1725.5 cm⁻¹, 1745.8 cm⁻¹, 1774.7 cm⁻¹) have been measured relative to those in the 2800-cm⁻¹ band (2819 cm⁻¹, 2826 cm⁻¹). A dual channel tunable diode laser system coupled to an astigmatic multipass cell was used to measure simultaneous transmission spectra in both the well-characterized 2800 cm⁻¹ and the previously unquantified 1740 cm⁻¹ bands. The line positions of the H₂CO absorptions in the 1740 cm⁻¹ band were determined by high-resolution FTIR measurements.

These line strengths were used during two field campaigns to quantify H₂CO concentrations, using tunable diode laser absorption spectroscopy at 1774 cm⁻¹. Measurements of the ambient concentration of H₂CO in Mexico City will be presented, along with measurements of the direct emissions from mobile sources. These results will be compared to the direct emission ratios of H₂CO coming from compressed natural gas (CNG) powered vehicles.

Infrared Laboratory Measurements of HCN Broadened by N₂ and Air

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Hydrogen cyanide. HCN. is now recognized as an important indicator of biomass burning emissions and is readily measured in infrared atmospheric spectra, though its spectral parameters have not been updated for over a decade. In this paper, we report preliminary results from analysis laboratory measurements of HCN broadened by N₂ and air as a function of temperature based on 0.01-cm⁻¹ resolution Fourier transform spectra recorded with lean mixtures. The measurements cover both the ν_1 and ν_2 bands from room temperature to temperatures as low as -60C. Improved broadening coefficients and pressure shift coefficients as a function of temperature are being derived from the spectra with the global fitting technique. Examples of the application of the new parameters to atmospheric measurements will be presented.

Vibrational Dependence of Broadening and Shift Parameters for Linear Molecules

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For a number of atmospheric molecules, enough measurements of broadening and pressure-induced shift parameters have accumulated in the literature so that we can begin to compare measurements in various vibration-rotation bands. While the vibrational dependence of pressure-induced line shifts is quite obvious, differences in broadening parameters between vibration-rotation bands are not so apparent, and they may be masked by the uncertainties and/or systematic errors in the measurements. Examples are given from our own recent work and from other published studies for three linear molecules: carbon monoxide (CO), carbon dioxide (CO₂), and hydrogen cyanide (HCN).

Extrapolation of Experimental Line-Width Data to Higher Rotational Quantum Numbers in the Case of Linear Molecules as Applicable to the Atmosphere

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Even if the data obtained in all of the laboratories of the world are fused together in order to generate an extensive and accurate database on air-broadened half-widths of infrared lines of any molecule, we would always find that the data did not extend to lines with high rotational quantum numbers, especially lines that are too weak to be observed in the laboratory but are of significance in atmospheric applications. So, in the absence of solidly founded and reliably accurate theories of collision-broadening, empirical extrapolation schemes are often advanced. Most of these schemes invoke polynomial fits. Using the extensive line-width, $\gamma^0(m)$, data measured in our laboratory on infrared lines of CO, CO₂, and N₂O at several temperatures between 200 and 296K, we have devised the following highly accurate empirical formula for the extrapolation of the data to high rotational quantum numbers m : $\gamma^0(m) = (C_0 + C_1 * |m|) / (|m| + N)$, where C_0 , C_1 , and N are adjustable parameters, as an alternative to polynomial fits. It is not only more accurate than any of the hitherto known polynomial representations, but also matches the trend exhibited by the experimental data accurately.

Rotational Lineshape Parameters of Atmospheric Trace Species

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The determination of atmospheric concentration profiles using from the Earth Observing System Microwave Limb Sounder EOS-MLS will require knowledge of many trace gas rotational lineshape parameters. The primary linewidth measurements are currently underway using the millimeter and sub-millimeter wave spectrometer here at the Jet Propulsion Laboratory. The instrument is composed of a synthesized source signal passed twice through a free-space absorption cell equipped with a cooling jacket and thermally insulated windows. The progress for a number of molecules will be presented, including HCl, HO₂, BrO, O₃, CO, SO₂, and CH₃CN. Inter-comparisons of the parameters to analogous infrared and/or theoretical values will be made where possible.

Effects of Line Mixing Upon Spectroscopic Line Parameters in the R Branch of the 1-0 Band of CO

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Spectroscopic line parameters were determined for the R branch of the 1-0 band of $^{12}\text{C}^{16}\text{O}$ without the inclusion of line mixing by the fitting of five Kitt Peak self-broadened FTS spectra with up to 200 Torr simultaneously.¹ The fitting was accomplished by the multispectrum nonlinear least squares fitting technique.² Four spectra have been added to this fit with up to 500 Torr pressure. The effects of line mixing are clearly evident. With the overlapping lines, it is essential to include the entire R branch in a single fit in order to determine the continuum unambiguously. Inclusion of line mixing between nearest neighbors increased the derived self-broadened Lorentz line widths by up to 7 for most of the branch. A few lines at higher J had increased line widths. Without line mixing, the self-induced pressure shifts varied from -0.0042 to $+0.0005$ $\text{cm}^{-1}/\text{atm}$. Inclusion of line mixing decreases this range to -0.0037 to -0.0016 $\text{cm}^{-1}/\text{atm}$. The best parameters to report on the HITRAN database depend upon whether the user includes line mixing in the computations.

1. V. Malathy Devi, D. Chris Benner, M.A.H. Smith and C.P. Rinsland, *JQSRT* **60**, 815-824 (1998).

2. D. Chris Benner, C.P. Rinsland, V. Malathy Devi, M.A.H. Smith and D. Atkins, *JQSRT* **53**, 705-721 (1995).

Spectroscopic Study for an Airborne Image Interferometer for the Analysis of Combustion Products from Biomass Burning

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The determination of principal gas constituents coming from fires by means of airborne instrumentation could be of great importance both for their detection and for the better characterization and understanding of the combustion process of biomass burning. For this purpose an image interferometer working in the visible-near-infrared region, which measures some relevant gaseous components coming from biomass burning like CO, CO₂, O₂, O₃, NO_x, and water vapour and determines temperature, is under study. The HITRAN database used in FASCODE allows the better line selection for increasing instrument sensibility and a better line discrimination in the regions of overlapping. Regarding to temperature determination, HITRAN and FASCODE allowed the identification of the fine structure 0.1nm line separation of several lines which have a better sensitivity with respect to temperature variations. In particular, this behaviour is noticed for CH₄ lines between 2.390-2.340 μm which are placed inside the strong 2.2-2.5 μm atmospheric absorption band. For the CO₂, absorption lines around 1.6 μm the same behaviour is observed. In the visible region water-vapour lines in the 0.55-0.75 μm range are the most sensitive to temperature variations. Beside, simulations using FASCODE have shown that in the presence of high aerosol loading, there is a decreasing of the line depths. The aim of this exercise is to assess the main spectroscopic requirements for the realization of an image interferometer which is able to determine temperature and to characterize the main products coming from combustion.

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