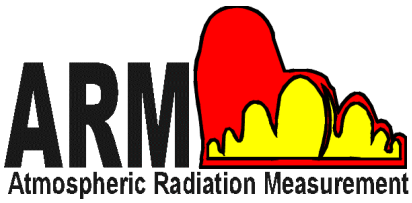
HITRAN DATABASE CONFERENCE

25TH ANNIVERSARY OF HITRAN

23-25 SEPTEMBER 1998



Air Force Research Laboratory
Space Vehicles Directorate/East
Science Center, Hanscom AFB MA

THE 5th BIENNIAL HITRAN DATABASE CONFERENCE
25TH ANNIVERSARY OF HITRAN

23-25 September 1998
AFRL/VS-East
Science Center

Wednesday, 23 September

8:00	Registration	
8:45	Opening	Hardy
9:00	Keynote	Goody
		Rothman
10:00	Break	
10:30	Session I: Molecules and Cross-sections	
		Upschulte
		Gamache
		Tashkun
12:00	Lunch	
1:30		Fukabori
		Dana
		Yoshino
3:00	Break	
3:30		Perrin
		Flaud
		Varanasi

Thursday, 24 September

9:00	Session II: Line Mixing	
		Benner
		Hartmann
10:00	Break	
10:30	Session III: Databases	
		DeLucia
		Husson
		Gasster
12:00	Lunch	
1:30	Special Address - Dan Hastings, Chief Scientist US Air Force	
1:45	Poster Session	

Friday, 25 Sept.		
9:00	Session IV: Aerosols	
		Massie
		Schroeder
10:00	Break	
10:30	Session V: Applications	
		Newnham
		Steinfeld
		Morrison
12:00	Lunch	
1:30	Panel meeting	

Final agenda to be completed later

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KEYNOTE SPEAKER:

Richard Goody

Richard Goody was born in 1921 in England. All of his studies took place at Cambridge University where he was from 1939 to 1953 with an absence of four years in World War II. He completed his Ph.D in 1949 and, from 1950 to 1953, was a Research Fellow at St. John's College.

From 1953 to 1958 he was Reader in Meteorology at the Imperial College of Science and Technology in London. In 1958 he joined Harvard University as Director of the Blue Hill Observatory and Professor of Dynamical Meteorology. Subsequently he was Professor of Planetary Physics and Applied Physics, Director of the Center for Earth and Planetary Physics, and has been Emeritus since 1991.

Richard Goody was elected to the American Academy of Arts and Sciences in 1959, to the National Academy of Sciences in 1970, and to the American Philosophical Society in 1997. He has received the Buchan Prize of the Royal Meteorological Society, the Cleveland Abbe Award from the American Meteorological Society, the Public Service Medal from NASA, and the William Bowie Medal from the American Geophysical Union.

He is the author of 5 books and 110 reviewed articles. His book, "Atmospheric Radiation, Vol. I Theoretical Basis," published in 1964, had a seminal impact on the creation of the HITRAN database. Since retirement he has written books and articles from his home in Falmouth, MA, and has spent a proportion of his time as a consultant to the Jet Propulsion Laboratory, and teaching at MIT and Caltech.

HITRAN INTO THE NEXT MILLENIUM

Laurence S. Rothman
AFRL/VSBM, 29 Randolph Road
Hanscom AFB MA 01731-3010

Barely more than a century has passed since the paper[1] by Arrhenius on the effect of CO_2 increase on the Earth's climate. A quarter of a century has elapsed since the distribution of the first HITRAN database.[2] As the second millenium draws to a close, scientists now have the tools to perform remote sensing experiments and calculations of radiance and transmission in atmospheres to an unprecedented degree of power.

This presentation reviews the history and progress that has been made in the HITRAN database in terms of increased spectral coverage, molecules and isotopomers, spectroscopic parameters, and media distribution. Suggestions for future work and directions will be presented.

1. S. Arrhenius, "On the Influence of Carbonic Acid in the Air upon the Temperature of the Ground," The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science. [Fifth Series] April 1896.
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The current effort has been supported by the US Air Force Office of Scientific Research; the NASA Earth Observing System (EOS), contract NAS5-96023; and the Atmospheric Radiation Measurement (ARM) program of the Environmental Sciences Division, Office of Biological and Environmental Research, US Department of Energy.

LINE STRENGTHS AND BROADENING PARAMETERS OF WATER BETWEEN 300-1000K NEAR 1.31 mm

Bernard L. Upschulte
Physical Sciences Inc.
20 New England Business Center
Andover MA 01810

Tunable DFB InGaAsP diode lasers were utilized to determine water line strengths and self broadening parameters of selected transitions between 7600 and 7640 cm^{-1} at temperatures up to 1100 K. The measured line strengths are compared with HITRAN96 and HITEMP96 databases. Measured line strengths for six groupings of lines between 300 and 1100 K agree to within 30 % with HITEMP96. Self-broadening coefficients and their temperature dependence were measured on four lines and compared with theoretical predictions.

COMPLEX ROBERT-BONAMY CALCULATIONS OF THE HALFWIDTH AND LINE SHIFTS OF ROTATION BAND TRANSITIONS OF H_2O AND O_3 PERTURBED BY N_2 AND O_2

Robert R. Gamache
Dept. of Environmental, Earth, and Atmospheric Sciences
University of Massachusetts Lowell
1 University Avenue, Lowell MA 01854

In this paper, complex Robert-Bonamy (CRB) calculations of the pressure-broadened halfwidth and pressure-induced line shift of two transitions of water vapor and one transition of ozone are reported. Calculations are made at temperatures in the range 200-400K for the 203.4 GHz transition of the $H_2{}^{16}O$, the 325.1 GHz transition of $H_2{}^{18}O$, and the 500.4 GHz line of $^{16}O_3$. The assumed intermolecular potential is a combination of electrostatic and atom-atom components. This last contribution is defined as the sum of pair-wise Lennard-Jones 6-12 interactions between the atoms of H_2O or O_3 and the atoms of the perturbing molecules, expanded to 8^{th} order. The calculated halfwidths and their temperature dependence are compared with measurement. Calculated and experimental results are in good agreement, within ±3.2%, except for the N_2-broadening temperature coefficients, for which there are discrepancies as high as 23%.

CDSD: A HIGH-PRECISION HIGH-TEMPERATURE SPECTROSCOPIC DATABANK OF THE CO_2 MOLECULE

Sergei A. Tashkun, Valery I. Perevalov
Institute of Atmospheric Optics, Siberian Branch, Russian Academy of Sciences
1, Akademitcheskii av., Tomsk 634055
RUSSIA

Jean-Luc Teffo
Laboratoire de Physique Moléculaire et Applications, CNRS,
Université Pierre et Marie Curie, case courrier 76, Tour 13, 4, place Jussieu
75252 Paris Cedex 05
FRANCE

The CDSD (Carbon Dioxide Spectroscopic Databank) databank is a high-precision, high-temperature spectroscopic databank of the CO_2 molecule. It covers the 15μm-0.6μm spectral range. The bank contains data for $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$, $^{16}O^{12}C^{17}O$, $^{16}O^{13}C^{18}O$, $^{16}O^{13}C^{17}O$, $^{13}C^{18}O_2$, $^{17}O^{12}C^{18}O$, $^{12}C^{17}O_2$, $^{13}C^{17}O_2$, $^{17}O^{13}C^{18}O$, and $^{12}C^{18}O_2$ isotopic species. The size of the databank depends on the intensity cutoff and may reach several Gigabytes.

The CDSD is based on the sets of effective Hamiltonian and effective dipole-moment operator parameters derived from the global fits of observed line positions and line intensities.[1,2] The latest global fit of essentially enlarged, recalibrated and cleaned set of more than 16000 observed line positions belonging to more than 200 vibrational bands of the $^{12}C^{16}O_2$ isotopic species enabled us to reach near measurement accuracy for the line positions: ~1MHz for laser heterodyne measurements, ~0.0002-0.001 cm-1 for Fourier-transformed measurements, and ~0.0005-0.005 cm^{-1} for flame emission spectra measurements. The global fits of more than 5000 observed line intensities of 120 vibrational bands of $^{12}C^{16}O_2$ covering the ν_2, $3\nu_2$, $5\nu_2$, $7\nu_2$, $9\nu_2$, and $11\nu_2$ regions led to standard deviations from 2% to 10% depending on the region. The standard deviations of the fits of other isotopic species of CO_2 are close to the experimental accuracies both for line positions and line intensities.

A comparison of CDSD and the CO_2 data in HITRAN-96 (Ref.3) databank will be presented. The largest differences between CSDS and HITRAN-96 data are connected with the Coriolis and l-type vibration-rotation interacting bands. The main goal of the creation of the CDSD databank is to supply precise data to researchers studying the Earth and planetary atmospheres, industrial combustion processes, space and aircraft engine exhausts.

1. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, L.S. Rothman, and Vl.G. Tyuterev, *JQSRT* **60,** in press (1998).
2. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, and Vl.G. Tyuterev, *JQSRT*, in press.
3. L.S. Rothman, R.R. Gamache, R.H. Tipping, C.P. Rinsland, M.A.H. Smith, D.C. Benner, V.Malathy Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S.T. Massie, L.R. Brown, and R.A.Toth, *JQSRT* **48,** 469 (1992).

MEASUREMENTS OF THE LINE STRENGTHS AND HALF-WIDTHS OF THE (2-0) AND (3-0) BAND OF CO

Masashi Fukabori, T.A. Aoki, T.E. Aoki
Meteorological Research Institute, Tsukuba,
Ibaraki 305-0052
JAPAN

H. Ishida and T. Watanabe
Toray Research Center Inc., Otsu,
Shiga 520-0842
JAPAN

In order to examine the uncertainties of the line parameters of the spectroscopic database, the absorption spectra of the (2-0) and (3-0) bands of CO in the near infrared region were measured with a high-resolution Fourier transform spectrometer at room temperature. The line strengths and half-widths of CO were determined by a nonlinear least squares technique. We compared our results with the values compiled in the HITRAN databases. The measured line strengths agreed well with the values of HITRAN92 and HITRAN96 within the experimental error for the (2-0) band of CO. The measured line strengths were 5% smaller than the HITRAN values for the (3-0) band of CO. The vibration-rotation coupling functions of these bands were obtained and the coefficients of the Herman-Wallis factors were compared with the values reported by other investigators. Self-, N_2-, and O_2-broadened half-widths were measured, and air-broadened half-widths were calculated with these values. We found that self-broadened half-widths of CO deviates from the values of HITRAN96, while air-broadened half-widths of CO were very close to the HITRAN96 values.

NO AND NO_2 NEW LINE PARAMETERS FOR THE NEXT HITRAN EDITION

Victor Dana, Jean-Yves Mandin, Mohamed-Yazid Allout
Laboratoire de Physique Moléculaire et Applications, UPR 136 du CNRS,
Université Pierre et Marie Curie, case courrier 76, Tour 13, 4, place Jussieu
75252 Paris Cedex 05
FRANCE

Alain Barbe, Laurence Régalia
Groupe de Spectroscopie Moléculaire et Atmosphérique, CNRS
Faculté des Sciences, BP 347
51062 Reims Cedex
FRANCE

and

Laurence S. Rothman
AFRL/VSBM, 29 Randolph Road
Hanscom AFB MA 01731-3010

This work presents improvements for the line parameters of NO and NO_2. The intensities and air-broadening coefficients of both NO and NO_2 are needed to determine the amount of nitrogen oxides present as pollutants in the urban lower troposphere. Furthermore, accurate line positions and line intensities involving high-v NO levels are needed to deduce the NO density in the lower thermosphere.

The great difficulties encountered for the involved molecules in retrieving some essential data from the experimental material will be discussed: presence of impurities in the samples, lines appearing as L-doublets for NO, or spin-rotation doublets for NO_2, very crowded spectra leading to numerous line overlappings for NO_2, non-negligible hyperfine splittings for NO, decomposition of NO when measuring the O_2-broadening parameters of NO lines, etc.

The main changes and improvements of HITRAN that will be presented are: New air-broadening coefficients of NO_2 lines in the spectral region of the $\nu_1+\nu_3$ band, obtained using an empirical formula deduced from our measurements, in place of the unique default value which is present in the current HITRAN version, and which can depart up to 20 % from our proposed values for some lines observable in the atmospheric window around 2900 cm^{-1}; A synthetic spectrum of the 2-0 and 3-1 bands of NO, based upon new measurements of line positions (including accurate L-splittings), line intensities, and N_2- and O_2-broadening coefficients

THE APPLICATION OF A VUV-FT SPECTROMETER AND SYNCHROTRON RADIATION SOURCE TO MEASUREMENTS OF THE NO AND O_2 BANDS

Kouichi Yoshino, James R. Esmond, William H. Parkinson
Harvard-Smithsonian Center for Astrophysics
60 Garden Street, MS-50, Cambridge MA 02138

Anne P. Thorne, J.E. Murray, G. Cox, R.C.M. Learner
Imperial College of Science, London, U.K.

K. Ito, T. Matsui
Photon Factory, KEK, JAPAN

T. Imajo
Kyushu University, JAPAN

K.W.-S. Leung and A.S.-C. Cheung
University of Hong Kong, Hong Kong

The Imperial College VUV-FT spectrometer has been equipped with optically contacted, beam splitters made from single crystals of MgF_2 and the short wavelength performance has been demonstrated down to ~139nm. To make ultra high resolution VUV photoabsorption cross section measurements with the VUV-FTS require 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 the NO and O_2 bands in the wavelength region 160-195 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 $A^2\Sigma^+ - X^2\Pi$ (3,0) and the $B^2\Pi - X^2\Pi$ (6,0), (9,0) bands of NO will be presented. The Schumann-Runge bands of O_2 have been also analyzed for the band with $v \geq 10$ in the wavelength region 175-183 nm. Absolute band oscillator strengths from the integration of cross sections of individual line have been obtained.

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. We also acknowledge the support of the Paul Instrument Fund of the Royal Society for the development of the UV-FT spectrometer. The FTS measurements at the Photon Factory were made with the approval of the Photon Factory Advisory Committee (94G367). KY thanks the Japan Society for the Promotion of Science for support.

NO_2 AND SO_2 LINE PARAMETERS: 1996 HITRAN UPDATE AND NEW RESULTS

Agnès Perrin, Jean-Marie Flaud
Laboratoire de Photophysique Moléculaire, CNRS
Université Paris Sud, Bât. 210, Campus d'Orsay
F-91405 ORSAY Cedex
FRANCE

Aaron Goldman
University of Denver
Department of Physics, 2112 E. Wesley Ave
Denver CO 80208

Curtis P. Rinsland
Atmospheric Sciences Division, NASA Langley Research Center
Hampton VA 23681-0001

Walter J. Lafferty
Optical Technology Division,
National Institute of Standards and Technology
Gaithersburg MD 20899

Claude Camy-Peyret and Philip Arcas
Laboratoire de Physique Moléculaire et Applications, CNRS
Université Paris Sud, Bât. 350, Campus d'Orsay
F-91405 ORSAY Cedex
FRANCE

It is well known that nitrogen dioxide, a minor constituent in the stratosphere, plays an important role in the chemical reactions controlling the concentration of ozone in the stratosphere. Sulfur dioxide is well known to be of astrophysical importance and plays an important role in the chemistry of planetary atmospheres. The terrestrial atmospheric opacity can be severely affected by volcanic eruptions, such as the recent events of Mt Pinatubo or El Chichon have demonstrated. On Venus, atmospheric SO_2 has been considered to be an indication of recent volcanic activity and is the major source of the H_2SO_4 cloud layer which encompasses the entire planet. This paper presents recent progress concerning the line positions and line intensities for these two molecules. Also, some recommendations for future work will be given.

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[1] "NO_2 and SO_2 line parameters: 1996 HITRAN update and new results," A. Perrin, J.-M. Flaud, A. Goldman, C. Camy-Peyret, W.J. Lafferty, Ph. Arcas, and C.P. Rinsland, *JQSRT* **60,** in press (1998).

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THE FAR INFRARED AND MID-INFRARED SPECTRUM OF HOCl

Jean-Marie Flaud
Laboratoire de Photophysique Moléculaire, CNRS
Université Paris Sud, Bât. 210, Campus d'Orsay
F-91405 ORSAY Cedex
FRANCE

Manfred Birk, Georg Wagner
DLR, Institut für Optoelektronik
D-82234 Oberpfaffenhoffen
GERMANY

Johannes Orphal
Institute of Environmental Physics
University of Bremen, P.O. Box 330440
D-28334, Bremen
GERMANY

Stefan Klee
Justus Liebig Universität
Heinrich Buff Ring 58
D-35392, Giessen
GERMANY

Walter J. Lafferty
Optical Technology Division,
National Institute of Standards and Technology
Gaithersburg MD 20899

The far infrared spectrum of HOCl has been recorded at high resolution between 20 and 360 cm^{-1} by means of Fourier transform spectroscopy, and it was possible to observe pure rotation lines involving rotational levels with high K_a quantum numbers (up to K_a = 9). These lines together with microwave and tunable-laser far infrared data were fitted leading to precise sets of rotational and centrifugal distortion constants for the ground states of both chlorine isotopomers. In addition, relative line intensities were measured permitting the determination of rotational corrections to the b-component of the permanent transition moment. Finally, to obtain Hamiltonian constants consistent with the newly determined ground state constants for the (100), (010) and (001) vibrational states, available data of the ν_1, ν_2 and ν_3 bands were refitted. Three interesting points are to be stressed. For the (001) state, we were able to complete the existing data with rotational lines observed in our spectra up to K_a values = 7. For $HO^{35}Cl$, we were able to show that some (010) and (100) levels are perturbed by levels of the (002) and (030) states respectively through Coriolis-type interactions. In this way, the band centers of these two dark states were determined.

ABSORPTION CROSS-SECTIONS OF HALOCARBONS

Prasad Varanasi
Institute for Terrestrial and Planetary Atmospheres
State University of New York at Stony Brook
Stony Brook NY 11794-5000

The need for the accurate parameterisation of the thermal infrared spectra of the most widely used chlorofluorocarbons (CFCs) and other halocarbons in the assessment of their global warming and ozone depletion potentials has been fairly well documented and discussed in recent publications and related conferences. The monitoring of the atmospheric concentrations of these chemicals by infrared remote sensing observations requires an accurate spectroscopic database of thermal infrared absorption cross-sections based upon carefully performed laboratory measurements. Our laboratory has been active for the past eight years in providing the necessary spectroscopic data to several international groups engaged in atmospheric remote sensing missions that employ balloon-borne and satellite-borne spectroscopic instruments. The retrievals of the vertical mixing ratios of CFCs and their alternates in these missions, most of which were in the solar-occultation mode, using our laboratory data have been termed highly successful. Our data have also become parts of the HITRAN and GEISA databases.

LINE MIXING IN METHANE AND APPLICATION TO HITRAN

D. Chris Benner
Department of Physics, College of William and Mary
P. O. Box 8795
Williamsburg VA 23187-8795

Mary Ann H. Smith, Curtis P. Rinsland
Atmospheric Sciences Division, Mail Stop 401A
NASA Langley Research Center
Hampton VA 23681-2199

Guy Guelachvili
Laboratoire de Physique Moléculaire et Applications, CNRS
Université Paris-Sud, Batiment 350, 91405 Orsay-Cedex
FRANCE

and

Linda R. Brown
Jet Propulsion Laboratory, California Institute of Technology
Pasadena CA 91109

Atmospheric spectral calculations in the 3000 cm^{-1} region using the HITRAN methane parameters are inadequate for experiments such as the Halogen Occultation Experiment (HALOE). Voigt parameters cannot simulate the spectrum for all pressures and temperatures present in the Earth's atmosphere. The inclusion of line mixing solves this problem, but the Rosenkrantz approximation is not sufficiently accurate. The fitting of a wide variety of methane laboratory spectra with temperatures from 210K to 296K, self and air broadening, and a wide range of path lengths and broadening pressures is displayed. The spectra are fitted with the multispectrum nonlinear least squares technique.[1] The fitted residuals are almost two orders of magnitude smaller than the best that can be done with only Voigt profiles. The challenge will be how to present the derived relaxation matrix element coefficients for the traditionally line-by-line HITRAN format.

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TOWARDS STORAGE OF LINE-MIXING PARAMETERS IN DATABASES

Jean-Michel Hartmann
Laboratoire de Physique Moléculaire et Applications, CNRS
Université Paris-Sud (bât. 350)
91405 Orsay Cedex
FRANCE

The need to account for line mixing effects in computations of atmospheric spectra (in some spectral regions) is now well established. This has stimulated numerous laboratory research works in the case of CO_2 Q branches which are strongly affected and often used for T/P retrievals. These studies are now being extended to other species (N_2O, CH_4, ...) whose spectra also show interference between lines at atmospheric pressures. Due to these efforts more and more data+models are available in the literature for the modeling of line-mixing effects and time has come for their gathering in databases. A number of solutions can be considered in order to model line-mixing effects on infrared spectra for practical applications. They involve different numerical data to be stored and require more or less complicated changes in atmospheric transmission/emission computer codes. Furthermore, in some cases, great care should be taken in order not to misuse these data and to avoid unphysical results such as negative radiances.

In any case, solution to the storage of line-mixing data should simultaneously consider the following problems: (1) It should be adapted to any absorbing species. (2) It should minimize the amount of data to be stored. (3) Update and changes resulting from a modification of some other database parameters should be easy to make. (4) It should require minimum changes of computer codes for their integration. (5) It should minimize the risks and consequences of misuse.

In the present paper, different solutions are considered and discussed in view of the five preceding constraints. Two approaches are retained based on storage of line-mixing parameters with some associated software. Their advantages and disadvantages are discussed and solutions for practical implementation in the current databases and computer codes are proposed.

MILLIMETER/SUBMILLIMETER SPECTROSCOPY AND THE ROTATION/VIBRATION DATABASE

Frank C. De Lucia
Department of Physics
174 W. 18th Avenue
Ohio State University
Columbus OH 43210

and

Paul Helminger
University of South Alabama

For a number of years the growth in resolution and measurement accuracy in the infrared, combined with the increased spectral coverage of microwave spectroscopy have made the development of integrated rotation/vibration databases advantageous. This talk will focus on the complementarity of these data sources and provide explicit examples.

THE 1997 SPECTROSCOPIC GEISA DATABANK SYSTEM

Nicole Jacquinet-Husson
LMD/CNRS
Ecole Polytechnique
Route Départementale 36
Palaiseau, Essonne 91128
FRANCE

The current version GEISA97 of the computer accessible system GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphérique: Management and Study of Atmospheric Spectroscopic Information) is described. This catalog contains 1,346,266 entries. These are spectroscopic parameters required to describe adequately the individual spectral lines belonging to 42 molecules (96 isotopic species) and located between 0 and 22,656 cm^{-1}. The featured molecules are of interest in studies of the terrestrial as well as the other planetary atmospheres, especially those of the Giant Planets. GEISA97 contains also a catalog of absorption cross-sections of molecules such as chlorofluorocarbons which exhibit unresolvable spectra. The modifications and improvements made to the earlier edition (GEISA92) and the data management software are described.

GEISA97 and the associated management software are accessible from the ARA/LMD (Laboratoire de Météorologie Dynamique du CNRS, FRANCE) Web site: http:ara01.polytechnique.fr/registration

INTRANET ACCESS TO THE HITRAN DATABASE

Samuel D. Gasster and Jeffery Collins
Radar and Signal Systems Department
The Aerospace Corporation
M4-927, P.O. Box 92957
Los Angeles CA 90009-2957

The HITRAN database (DB) has gained wide use within the scientific community over the past 25 years. There are many diverse applications for this database within our company. Scientists and engineers involved with both fundamental and applied aerospace and remote sensing research access the HITRAN DB data over the full spectral range from the microwave to the ultraviolet. With so many users dispersed throughout our company, we decided to develop and demonstrate a centralized capability to access the HITRAN DB via our corporate intranet. The primary advantage is that we can now maintain a single up-to-date central access point for the HITRAN data.

The HITRAN DB is accessed by the user via a standard sequence of HTML forms to build a query for the DB. The user submits the forms to the HTTP server (Apache 1.3) which then processes the request via a CGI application program written in Python. The Python CGI performs the interface to the HITRAN DB, any physical computations using HITRAN DB data to user specified values (e.g., temperature scaling of line strengths and widths), and handles output formatting. To simplify database queries we have imported the standard HITRAN DB into mSQL, a lightweight structured query language server. The results of the HITRAN DB query can be output in various formats depending on the size of the data. For relatively small query results the data are returned directly to the user's browser as HTML, and for larger query results the data are saved to an ASCII flat file accessible via ftp.

This paper will summarize the development and performance of our tool to access HITRAN using our corporate intranet.

INDICES OF REFRACTION FOR ATMOSPHERIC REMOTE SENSING

Steve Massie
NCAR, PO Box 3000
Boulder CO 80307

and

Aaron Goldman
Department of Physics
University of Denver
2112 E. Wesley Ave
Denver CO 80208

A review of the HITRAN indices of refraction for atmospheric remote sensing is presented. New indices of H_2SO_4/H_2O, the status of indices applicable for PSCs (Polar Stratospheric Clouds), and indices of water and ice are discussed. Atmospheric spectra from experiments (e.g. CRISTA) are presented, to illustrate how PSC and cirrus particles influence atmospheric emission in the infrared.

FREQUENCY AND TEMPERATURE DEPENDENT MODELS FOR THE BULK OPTICAL CONSTANTS OF AEROSOLS

Michael E. Thomas, Matthew D. Banta
Johns Hopkins University, Applied Physics Laboratory
Laurel MD. 20723-6099

and

John Schroeder
Ontar Corp., 9 Village Way
N. Andover MA 01845-2000

A modified classical oscillator model is used to represent the optical constants of ice Ih and water as a function of frequency (80 to 7000 cm^{-1} for ice and from the microwave to the ultraviolet for water) and temperature. In addition to the modified classical oscillator model for phonon bands, other models are used to completely characterize the optical constants of NaCl, quartz, fused silica and other solids of interest.

SHORTWAVE RADIATIVE FORCING: OBSERVATIONS AND REQUIREMENTS FOR IMPROVED NEAR-INFRARED AND VISIBLE SPECTRAL DATA

David A. Newnham, A.E. Heathfield, Kevin M. Smith, and John Ballard
Space Science Department
Rutherford Appleton Laboratory
Chilton DIDCOT Oxon OX11 0QX
U.K.

Recent field measurements of the near-infrared and visible transmittance of solar radiation through the terrestrial atmosphere have been made using a ground-based, high-resolution Fourier transform spectrometer at RAL. These studies indicate limitations in the current molecular databases for the 2-micrometer to 400-nm spectral region. New laboratory studies using the RAL Molecular Spectroscopy Facility aim to address this problem by providing quantitative line, broadband, and aerosol scattering data for shortwave radiative forcing and remote sensing applications.

SPECTROSCOPIC DATABASE REQUIREMENTS FOR AIR QUALITY MONITORING AND REGULATION

Jeffrey I. Steinfeld, Matthew Gardner, Manjula Canagaratna, Sheng Fu Yang, Barclay Gibbs, Scott Witonski, and Teresa Raine
Department of Chemistry
G.R. Harrison Spectroscopy Laboratory, and Technology and Policy Program
Massachusetts Institute of Technology
Cambridge MA 02139

HITRAN and related atmospheric spectroscopy databases are a valuable resource for measurements on an important but relatively small set of atmospheric molecules. Making use of high-sensitivity spectroscopic techniques for tropospheric air quality measurements will require data on a much larger range of gas-phase species. The U.S. Environmental Protection Agency has identified 189 volatile organic compounds as high-priority Hazardous Air Pollutants (HAP's). Only two of these priority HAP's appear in the current HITRAN (HAWKS96) database, showing that a great deal of basic spectroscopic data remains to be accumulated and systematized for these substances. We will review the available data, possible measurement techniques, and regulatory issues for a selected set of HAP's, including methyl bromide, chlorinated ethylenes, dimethyl ether, acetone, formaldehyde, and chloroform.

Support for this work has been provided by the MIT - Swiss Federal Institutes of Technology - University of Tokyo Alliance for Global Sustainability, the Martin Fund for Environmental Studies, the Ford Consortium on Environmental Challenges, and the Dreyfus Postdoctoral Fellowship Program in Environmental Chemistry.

USING THE HITRAN DATABASE TO PERFORM QUANTITATIVE FTIR MEASUREMENTS OF GAS CONCENTRATIONS AND TEMPERATURES DURING CVD

Philip W. Morrison, Jr., Oranut Taweechokesupsin, Ram Raghavan, and Eric Szeto
Department of Chemical Engineering
Case Western Reserve University
Cleveland OH 44106-7217

In situ Fourier infrared (FTIR) spectroscopy can make a valuable contribution to the understanding of chemical vapor deposition (CVD) of thin films and fine particles. The main objectives of the gas phase measurements are the determination of the temperature and concentrations of the various stable and radical molecules found in the CVD reactor. Relative concentration measurements have been made in the past, but such measurements cannot be easily compared to numerical simulations of the reactive flow. Interpreting the measured spectra quantitatively is complicated by the large temperature gradients present in the reactor which can confuse the interpretation of the absorption spectra. One can address this problem by performing calibration measurements at various temperatures, but this method is impractical at the highest gas temperatures where even stable gas species react.

We circumvent this problem by using the HITRAN database to calculate the gas spectra at high temperatures. The first step is to calculate a high-resolution spectrum (better than 0.01 cm^{-1}) and then convolve it with the line shape function of the FTIR at the measured resolution (1 cm^{-1}). This method involves performing an inverse Fourier transform on the HITRAN spectrum to generate an interferogram, truncating and apodizing the interferogram to 1 cm^{-1} resolution, and then Fourier transforming back to the spectral domain. Unlike previous convolution methods, this method works on an entire gas band and can handle overlapping gas peaks. The local temperature used in the above calculation comes from in situ emission and transmission FTIR spectra which requires no prior knowledge of the concentrations.

Examples will be taken from hot filament CVD of diamond films, flame synthesis of TiO_2 particles in a CH_4/O_2 flame, and growth of diamond thin films using an oxyacetylene torch.

POSTER SESSION

UNB-NIST MOLECULAR SPECTROSCOPY DATA ACTIVITIES

Li-Hong Xu
University of New Brunswick
St. John, NB E2L 4L5
CANADA

and

Jon T. Hougen
NIST
Gaithersburg MD 20899

We have started to put ground state energy levels on the web for a number of small molecules exhibiting one or more large-amplitude motions, since such energy levels are often obtainable only from quite complicated spectral analyses and/or model Hamiltonians, not readily accessible to workers in fields outside high-resolution molecular spectroscopy. Initial plans include levels for CH_3OH, CH_3CHO, CH_3NH_2 and NH_2NH_2, which we have done some work on ourselves. We hope to obtain energy levels for H_2O_2 and CH_3CH_3 from other laboratories. In addition to the energy levels themselves, some discussion of the number and kind of large amplitude motions, the group theoretical symmetry species labels, selection rules, references, etc. will be given. Sample web-page printouts will be shown in the poster.

SPECIAL QUANTITATIVE SPECTROSCOPY ISSUES IN THE HITRAN 1996 LINE PARAMETERS

Aaron Goldman
Department of Physics
University of Denver
2112 E. Wesley Ave
Denver CO 80208

Critical reviews of specific molecules prepared for the 1996 ASA (Atmospheric Spectroscopy Applications) and 1996 HITRAN Special Issues of *JQSRT* (volume **59,** no. 3-5 and volume **60,** no. 5, respectively) show significant improvements in the quality and scope of the line parameters. However, there are also a number of special unresolved which include:

(i) Incomplete treatment of fine, hyperfine, isotopic, and high-v,J transitions which are important in atmospheric spectra (O_3, NO, HNO_3, HBr, HI,…).

(ii) Inconsistent band-to-band intensities from different spectral regions (OH, NO, HNO_3,…).

(iii) Misinterpretation of partition functions, statistical weights, and weighted transition probabilities for molecules with unique energy sub-level structure.

(iv) Incomplete coverage of cross-sections for heavy molecules needed for atmospheric P,T conditions.

Future work is planned to resolve these issues.

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[3] A. Goldman, L.R. Brown, M.N. Spencer, C. Chackerian, Jr., L.P. Giver, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin, "NO Line Parameters: Review of 1996 HITRAN Update and New Results," *JQSRT* **60,** in press (1998).

ANALYSIS OF JET ENGINE EXHAUST H_2O AND SO_2 SPECTRA

Joda Wormhoudt, Tim A. Berkoff, and Richard C. Miake-Lye
Aerodyne Research, Inc.
Billerica MA 01821-3976

Tunable diode laser infrared absorption spectra of the exhaust of an aircraft engine operating in an altitude test cell were analyzed using HITRAN line parameters for H_2O and SO_2, then re-analyzed using revised parameters from several very recently published studies. Our goal is measurement of emitted SO_2 per unit of fuel burned, a quantity known as the emission index. Since there is a direct relationship between fuel consumption and water emission in the exhaust, the ratio of SO_2 and H_2O line intensities can, in principle, give us the emission index directly. In practice, the SO_2 and H_2O lines we measured have different temperature behaviors, and a knowledge of the line parameters is needed to derive an accurate SO_2 emission index. We will present examples of the effects of changing line parameters on the values we derive, as well as an estimate of the contribution of uncertainties in line parameters to the overall error limits of our measurement.

LINE-PARAMETER MEASUREMENTS OF STRONGER WATER-VAPOR LINES IN THE 1.5- AND 1.9-mm REGIONS

Robert L. Hawkins
Air Force Research Laboratory
AFRL/VSBM, 29 Randolph Road
Hanscom AFB MA 01731-3010

and

Bill Phillips
Sverdrup Technology, 1099 Avenue C
Arnold AFB TN 37389-9013

Many of the strongest water vapor lines in the 1.5- and 1.9-μm regions have not been updated in the HITRAN listing since before HITRAN86. (Lines of medium strength in the 1.5-μm region were updated more recently, using the measurements of Toth[1].) Recently, 0.008 cm^{-1} resolution Fourier transform spectra of water vapor in these regions have been measured. Some 733 absorption lines were identified and fit by nonlinear least-squares, yielding line positions, intensities, and self-broadening coefficients. While knowledge of water vapor in this region remains incomplete, these new line parameters represent a significant improvement.

1. R.A. Toth, "Extensive measurements of $H_2{}^{16}O$ line frequencies and strengths: 5750 to 7965 cm^{-1}," *Appl. Opt.* **33,** 4851-4867 (1994).

HIGH TEMPERATURE SPECTRUM OF H_2O IN THE 720 TO 1400 cm^{-1} REGION

Mark P. Esplin, Richard B. Wattson
Stewart Radiance Laboratory, Utah State University
139 The Great Road
Bedford MA 01730

Michael L. Hoke and Laurence S. Rothman
Air Force Research Laboratory
AFRL/VSBM, 29 Randolph Road
Hanscom AFB MA 01731-3010

Spectral line positions[1] and line position uncertainties have been determined for 1605 absorption lines of H_2O in the spectral region from 720 cm^{-1} to 1400 cm^{-1}. Transition identifications were confirmed for 921 of these 1605 spectral lines. The line-position measurements were obtained from a co-added transmittance spectrum having a signal-to-noise ratio greater than 100 to 1. The apodized spectral resolution was 0.009 cm^{-1}. The 20 Torr H_2O sample was heated to approximately 1000K, in a 1.75-meter single pass sample cell. The wavelength scale of the transmittance spectrum was calibrated by using strong well-known H_2O spectral lines. The line-position estimates and identifications were checked using a modified Loomis-Wood diagram technique. Initial guess line-position estimates were obtained from either HITRAN92 or a direct numerical diagonalization (DND) calculation of the H_2O Hamiltonian. The transition identifications were confirmed and a consistent set of line-position values determined using a combination-difference technique to check closed loops on an energy level diagram. A few large (>0.1 cm^{-1}) and many smaller (from 0.1 to 0.001 cm^{-1}) line position differences were found when the measured line positions were compared to the values on HITRAN92. These differences are all larger than the line-position measurement uncertainties, which are generally less than 0.001 cm^{-1}. All of the new and confirmed H_2O line-position measurements have been incorporated into HITRAN96.

1. M.P. Esplin, R.B. Wattson, M.L. Hoke, and L.S. Rothman, *JQSRT* **60,** in press (1998).

DIRECT NUMERICAL DIAGONALIZATION LINE-BY-LINE CALCULATIONS COMPARED TO LINE PARAMETERS IN SEVERAL WEAK INTERACTING CO_2 BANDS NEAR 7901 cm^{-1}

Richard B. Wattson
Stewart Radiance Laboratory
Bedford MA 01730

Lawrence P. Giver, Rohidas J. Kshirsagar, Richard S. Freedman, and Charles Chackerian, Jr.
NASA Ames Research Center
Moffett Field CA 94035

The recent measurements of the $2\nu_3$-series perpendicular bands of CO_2, done by the AMES group, leave only perturbed bands with important updates in line positions and intensities to be done, for HITRAN at least. The present line parameters for perturbed bands on HITRAN are from very old data that have been shown to have some serious errors. Work has progressed with the calculation, by direct numerical diagonalization (DND),[1] for the next HITRAN database using a line-by-line approach instead of the band-by-band approach that has been used in the past. A new dipole-moment surface, incorporating the $2\nu_3$ series, has also been determined.

The 7901 cm^{-1} band, (21122-00001), is particularly interesting as it is a perturbed band and also a member of the $2\nu_3$ series of perpendicular bands. It is the principal band in determining an important near-IR window region in Venus dark-side emission. While the calculation of line intensities by DND has normally proven to be of high reliability, some data suggest that the calculation of the Herman-Wallis parameters and sometimes even the band intensities by DND can be in error. Recent calculations have shown that the new line-by-line approach should correct these errors.

A substantial set of new CO_2 spectra from 4500 to 12000 cm^{-1} has been obtained at Ames with 1500 m path length using a Bomem DA8 FTS. The prior measurements of the 21122-00001 vibrational band at 7901 cm^{-1} were limited to Q- and R-branch lines; with improved signal/noise of these spectra some lines in the weaker P branch have now also been measured. The 21122 (G_v = 7901.48 cm^{-1}) levels are known to be perturbed by the 32211 (G_v = 7897.57 cm^{-1}) levels, and the new DND calculations predict that high-J lines of the forbidden 32211-00001 vibrational band "borrow" intensity from the corresponding transitions of the 21122-00001 band. We have identified such Q- and R-branch transitions of the 32211-00001 band from $26 < J'' < 44$, based on our position measurements of lines in the 32211-02201 band at 6562 cm^{-1}. Comparisons will be shown between the DND calculations of line parameters for these bands, with the present observations as an example of the DND capability for CO_2 predictions.

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LINE INTENSITY AND POSITION MEASUREMENTS AND DERIVED BAND PARAMETERS OF THE 31103-00001 $^{12}C^{16}O_2$ BAND AND ITS TWO NEARBY HOT BANDS

Lawrence P. Giver, Rohidas J. Kshirsagar, Richard S. Freedman, and Charles Chackerian, Jr.
NASA Ames Research Center
Moffett Field CA 94035

Richard B. Wattson
Stewart Radiance Laboratory
Bedford MA 01730

Linda R. Brown
Jet Propulsion Laboratory, California Institute of Technology
Pasadena CA 91109

A set of CO_2 spectra from 4500 to 4780 cm^{-1} has been obtained at Ames with 1500 m path length using a Bomem DA8 FTS. This spectral region contains a number of weak bands and minor isotopic bands that have been studied at high resolution in the reflection spectrum of Venus by Mandin.[1] Improved laboratory intensity and position measurements should assist modeling the Venus reflection spectra and improve understanding of Venus' upper atmosphere. Also, the laboratory measurements will assist DND intensity computations of weaker bands that cannot be measured, but which are nevertheless significant absorbers in Venus' deep, hot CO_2 atmosphere. For example, some of the weaker bands that are members of the same polyads as the bands in this presentation lie in the nearby 2.3-μm emission window[2] in Venus' night-side spectrum.

The spectra obtained at Ames had higher signal/noise than our prior spectra.[3] This was achieved in part by including a circular variable filter wheel limiting the band-pass of each spectrum to a few hundred wavenumbers. We re-measured P- and R-branch lines of the 31103-00001 vibrational band at 4591 cm^{-1} on these new spectra and also on several spectra obtained previously with shorter path lengths at Kitt Peak. Assignments, positions, and intensities of lines of the weak Q branch of this band were also determined from the Ames spectra. Q-branch lines of this band were previously observed, but misassigned, by Mandin in Venus' spectrum. The current HITRAN values of the rotational constants for the 31103f level are incorrect due to mis-assignments of Q-branch lines of the 31103-10002 band by Benner et al.[4] The rotational constants we have determined for the 31103f level are B=0.3913585, and $D=1.61\times10^{-7}$. The 31103-00001 rotationless band strength determined from these Q-branch line intensity measurements alone is $S_v^0 = 2.90\times10^{-25}$. This result is nearly identical to the current HITRAN value of $S_v^0 = 2.89\times10^{-25}$, which was previously determined from P- and R-branch measurements by Giver and Chackerian.[5]

The signal/noise of the Ames spectra was sufficiently high to measure positions and intensities of some R-branch lines of the 40004-01101 hot band at 4530 cm^{-1}, and both P- and R-branch lines of the 32203-01101 hot band at 4578 cm^{-1}. Results of these measurements will also be presented. Although too weak for inclusion in the HITRAN tabulation, these bands and other related bands are significant absorbers in the lower atmosphere of Venus.

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LINE STRENGTHS AND HALF-WIDTHS OF CO_2 IN THE 2.0-mm REGION

Masashi Fukabori, T.A. Aoki, T.E. Aoki
Meteorological Research Institute, Tsukuba,
Ibaraki 305-0052
JAPAN

H. Ishida and T. Watanabe
Toray Research Center Inc., Otsu,
Shiga 520-0842
JAPAN

Absorption spectra of CO_2 in the 2.0-micron region were measured with a high-resolution Fourier transform spectrometer at room temperature. The line strengths and half-widths were determined with a nonlinear least squares technique. The line strengths of the (20012-00001) band were close to the HITRAN96 values except for high-J lines in the R-branch. The line strengths of the (20011-00001) band were about 3% larger than the HITRAN96 values, and the line strengths of the (20013-00001) band were 5-10% smaller than the values of HITRAN96. Self- and air-broadened half-widths were about 5% larger than the values of HITRAN96.

The rotationless dipole-moment matrix element and the Herman-Wallis coefficients were also determined for each band.

BROADENING AND SHIFT COEFFICIENTS DUE TO AIR AND NITROGEN IN THE $2n_2^0$ AND n_1 BANDS OF $^{16}O^{13}C^{18}O$

V. Malathy Devi, D. Chris Benner
Department of Physics
The College of William and Mary
Box 8795
Williamsburg VA 23187-8795

Mary Ann H. Smith and Curtis P. Rinsland
Atmospheric Sciences Division, Mail Stop 401A
NASA Langley Research Center
Hampton VA 23681-2199

The first experimental measurements of the Lorentz broadening coefficients and pressure-induced shift coefficients due to air and nitrogen for 93 vibration-rotation lines in the $2\nu_2^0$ and ν_1 bands of $^{16}O^{13}C^{18}O$ are presented. The measurements extend from P(46) to R(46) and P(50) to R(45), respectively in the two bands. The results are obtained by analyzing ten long path, high-resolution laboratory absorption spectra recorded using a 90% ^{13}C-enriched sample of carbon dioxide at 0.0027 cm^{-1} resolution (800 cm^{-1} to 1400 cm^{-1} spectral region) using the McMath-Pierce Fourier transform spectrometer. A multispectrum nonlinear least-squares technique is used to determine the parameters.[1] The air-broadening coefficients obtained in this work agreed well with the values reported for the 29 $2\nu_2^0$ and 64 ν_1 band lines in the HITRAN database.[2] Nitrogen-broadening coefficients are 4% larger than the air-broadening coefficients. Similar to broadening coefficients, the pressure-induced shift coefficients are also transition dependent, but different for the P- and R-branch lines with the same J values. Except for a few R-branch lines, the shift coefficients are negative, and range between $+4\times10^{-3}$ cm^{-1}/atm at 296 K and -5.6×10^{-3} cm^{-1}/atm at 296 K. No significant difference in the pressure-induced shift coefficients for air and nitrogen is found. Comparisons of the broadening and pressure-induced shift coefficients between the two bands, between the P and R branches, and between the two broadening gases are made. The results are also compared with the values reported in the literature for the more abundant $^{12}C^{16}O_2$ molecule.

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INTENSITIES, BROADENING, AND SHIFT PARAMETERS IN THE FUNDAMENTAL BANDS OF OZONE

Mary Ann H. Smith, Curtis P. Rinsland
Atmospheric Sciences Division, Mail Stop 401A
NASA Langley Research Center
Hampton VA 23681-2199

D. Chris Benner, and V. Malathy Devi
Department of Physics
The College of William and Mary
Box 8795
Williamsburg VA 23187-8795

High-resolution Fourier transform absorption spectra of ozone have been recorded and analyzed to determine absolute intensities of $^{16}O_3$ lines in the 9-11 μm region.[1] The 254 nm UV-absorption absorption cross-section value of Mauersberger et al.[2] was used as a reference standard. A multispectrum nonlinear least-squares procedure[3] was used to fit four spectra simultaneously to determine intensities for 366 lines in the ν_3 fundamental band and 10 lines in the ν_1 band. The absolute accuracy of these intensity values ranges from 2 % for the strongest, most well-determined lines to 4 or 5 % for the weakest lines measured. On average, our measured intensities are approximately 1 % larger than the values on the current HITRAN compilation.[4] Comparison with other recent experimental studies shows excellent agreement for a few lines and adequate agreement (considering all possible sources of uncertainty and systematic errors) for the others.

High-resolution absorption spectra of ozone broadened by dry air were recorded at a number of temperatures from -63°C to 23°C. The multispectrum nonlinear least-squares procedure[3] was used to fit 29 of these spectra simultaneously to determine the air-broadening and shift coefficients and their temperature dependences for over 440 lines in the ν_1 band and over 350 lines in the ν_2 band.[5,6] Room-temperature self-broadening coefficients were also determined for most of the lines measured. In both bands we observed that the air- and self-broadening coefficients for transitions with $K_a'' = J''$ are much smaller than those obtained for other lines, and our retrieved temperature dependence exponents for air-broadening are significantly smaller than the mean value given in the HITRAN compilation.[4] We have recently recorded more air-broadened O_3 spectra at temperatures down to 165 K and are currently analyzing broadening and shift coefficients for lines in the ν_3 band.

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CO AS AN INTENSITY STANDARD IN THE REGION OF 4.7, 2.3 AND 1.5 mm

Charles Chackerian, Jr.
NASA Ames Research Center
MS 245-4
Moffett Field CA 94035-1000

Line intensities up to J = 25 of the 3 - 0 vibrational band of $^{12}C^{16}O$ have been determined from laboratory spectra recorded at Kitt Peak National Solar Observatory (KP) and the NASA Ames Research Center (NA). The KP and NA spectra were recorded with optical paths of 73 and 207 meters respectively and the individual intensity determinations agree to 1 % and better. Between J = 0 - 25 these results are 5 - 10% smaller than HITRAN1996. Once the electric-dipole moment function of CO is re-determined using these results, it is likely that larger effects will be seen in the higher v, $\Delta v = 3$ transitions.

MEASUREMENTS OF AIR-BROADENING AND PRESSURE-INDUCED SHIFT COEFFICIENTS, AND LINE MIXING IN THE 1000 TO 1300 cm^{-1} SPECTRAL REGION OF $^{12}CH_3D$

D. Chris Benner, V. Malathy Devi
Department of Physics
The College of William and Mary
Box 8795
Williamsburg VA 23187-8795

Mary Ann H. Smith and Curtis P. Rinsland
Atmospheric Sciences Division, Mail Stop 401A
NASA Langley Research Center
Hampton VA 23681-2199

Measurements of air-broadening and air-induced shift coefficients, relative intensities and accurate line positions are reported for $^{12}CH_3D$ lines between 1000 and 1300 cm^{-1}. In addition, line mixing effects are observed and values for relaxation matrix elements are obtained for the first time in several of the K″ = 3 A1A2 split lines in the ^{r}P, ^{p}P, ^{q}P, ^{r}Q, ^{p}Q, ^{p}R and ^{r}R sub-band lines in the ν_6 band. These results are obtained from analysis of eleven (0.005 cm^{-1} resolution) laboratory absorption spectra recorded with the McMath-Pierce Fourier transform spectrometer at the National Solar Observatory on Kitt Peak, Arizona. The data are obtained with a high purity (99%) isotopic sample of $^{12}CH_3D$. Two absorption cells with path lengths of 25 and 150 cm are used. Three low-pressure spectra using pure $^{12}CH_3D$ with 1 to 3 Torr and eight broadened spectra of dilute mixtures (~ 1%) of $^{12}CH_3D$ in dry air with total pressures between 100 and 400 Torr are used to determine the broadening and shift coefficients, and line mixing. A multispectrum nonlinear least-squares spectral fitting technique[1] is used in the analysis. The calibration of the wavelength scale of each spectrum is obtained relative to the positions of the ν_2 band water vapor lines published by Toth.[2] Results are compared with previous measurements and calculations.

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TEMPERATURE DEPENDENCE OF AIR-BROADENING COEFFICIENTS AND AIR-INDUCED PRESSURE-SHIFT COEFFICIENTS IN THE ν_3 AND $\nu_2+\nu_4$ BANDS OF $^{12}CH_4$

V. Malathy Devi, D. Chris Benner
Department of Physics
The College of William and Mary
Box 8795
Williamsburg VA 23187-8795

Mary Ann H. Smith, Curtis P. Rinsland
Atmospheric Sciences Division, Mail Stop 401A
NASA Langley Research Center
Hampton VA 23681-2199

Guy Guelachvili,
Laboratoire de Physique Moléculaire et Applications, CNRS
Université Paris Sud, Bâtiment 350, 91405 Orsay-Cedex
FRANCE

Linda R. Brown
Jet Propulsion Laboratory, California Institute of Technology
Pasadena CA 91109

Absorption spectra (0.01 cm^{-1} resolution) of a high purity natural sample of methane at low pressures (~1 Torr) as well as dilute mixtures of methane (~1%) in dry air (75 Torr to 450 Torr) were recorded at various temperatures (–600 C to 250 C) using the McMath-Pierce Fourier Transform Spectrometer of the National Solar Observatory on Kitt Peak, Arizona. The room temperature spectra were obtained using cells with path lengths of 5, 25, 150, and 2500 cm while the cool spectra were recorded using a 50 cm long Pyrex coolable cell. In addition, higher resolution (0.0027 cm^{-1}) absorption spectra of a pure sample of $^{12}CH_4$ at room temperature were obtained using the Fourier transform spectrometer at the Laboratoire de Physique Moléculaire et Applications at Orsay, France. Path lengths between 0.6 cm and 4 m and pressures from less than one Torr to more than 500 Torr were used in recording these spectra. The temperature dependence of the air-broadened halfwidth coefficients and pressure-induced line shift coefficients for over 250 transitions in the P branch side of the ν_3 band were determined. These results are obtained by analyzing more than 40 spectra simultaneously using a multispectrum nonlinear least-squares fitting algorithm.[1] Variations in the measured parameters with the symmetry species and the rotational quantum numbers of the transitions between the ν_3 and $\nu_2+\nu_4$ bands are discussed. Comparisons of the present results with previous measurements and calculations are made.

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INTENSITIES, WIDTHS AND SHIFTS OF OXYGEN AT 0.762 mm

Linda R. Brown
Jet Propulsion Laboratory
California Institute of Technology
Pasadena CA 91109

and

Claude Plymate
NOAO / National Solar Observatory
Tucson AZ 85726

SAGE III, an EOS remote sensing experiment scheduled to orbit the Earth, will utilize the prominent features of the oxygen A-band to monitor atmospheric pressure and temperature. To validate the oxygen line parameters, the intensities, pressure-broadened line widths and pressure-induced frequency shifts of the strongest transitions between 13040 and 13165 cm^{-1} have been measured using the McMath Fourier transform spectrometer located at Kitt Peak National Observatory / National Solar Observatory in Arizona. For wavenumber calibration, a broad band spectrum has been recorded between 4000 and 14000 cm^{-1}.

LABORATORY STUDIES OF SPECTRAL LINE PARAMETERS IN THE 10-MICRON BANDS OF AMMONIA

Vasilii Nemtchinov and Prasad Varanasi
Institute for Terrestrial and Planetary Atmospheres
The University at Stony Brook
Stony Brook NY 11794-5000

Infrared spectroscopic parameters of NH_3 are needed for the determination of ammonia concentration in the Jovian atmosphere from astronomical observations. Ammonia is also present in the interstellar medium and as a trace constituent is present in the Earth's atmosphere. Its spectral line parameters are also important for the accurate modeling of the longwave radiative transfer in the 10-μm region in terrestrial and planetary atmospheres. We present recent high-resolution studies of pressure-broadened half-widths of spectral lines in the ν_2 bands of ammonia performed in our laboratory. These data were obtained with low temperature absorption cells and a high-resolution Fourier transform spectrometer.

RECENT PROGRESS IN THE ANALYSIS OF HNO_3 SPECTRA

Agnès Perrin, Jean-Marie Flaud
Laboratoire de Photophysique Moléculaire, CNRS
Université Paris Sud, Bât. 210, Campus d'Orsay
F-91405 ORSAY, Cedex
FRANCE

Aaron Goldman
University of Denver
Department of Physics, 2112 E.Wesley Ave
Denver CO 80208

Curtis P. Rinsland
Atmospheric Sciences Division, NASA Langley Research Center
Hampton VA 23681-0001

Numerous studies of HNO_3 spectra have been performed recently in the infrared, far infrared or microwave regions leading to very significant improvements in the quantitative spectral parameters of HNO_3, i.e. line positions and line intensities. This paper will summarize recent results concerning either isolated or interacting IR bands of HNO_3 of atmospheric interest. These bands are, indeed, used for the atmospheric detection of HNO_3 by IR methods. Also, in order to get relevant parameters for the $3\nu_9-\nu_9$ hot band which appears to lead to significant absorption in stratospheric spectra (ATMOS) at 11 μm, the torsional splitting which affects mainly the ν_9 states, and which is due to the large amplitude motion of the H atom relative to the $O-NO_2$ frame, has to be taken into account explicitly.

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NEW LINE POSITIONS AND ABSOLUTE LINE INTENSITIES FOR THE FAR INFRARED AND ν_6 BANDS OF H_2O_2

Agnès Perrin, Jean-Marie Flaud
Laboratoire de Photophysique Moléculaire, CNRS
Université Paris Sud, Bât 210, Campus d'Orsay
F-91405 ORSAY Cedex
FRANCE

Stefan Klee and Manfred Winnewisser
Justus Liebig Universität, Physikalisch-Chemisches Institüt
Heinrich-Buff-Ring 58, D-35392 Giessen
GERMANY

The purpose of this work was to obtain reliable line positions and line-intensity parameters for two spectral ranges which can be used for remote measurements of hydrogen peroxide, namely the far infrared and the 7.9-μm regions which correspond to the torsion-rotation band and to the ν_6 band of H_2O_2 respectively. Two difficulties have to be faced: (1) H_2O_2 has a large amplitude torsional motion of the OH bond relative to the O-O bond; (2) H_2O_2 decomposes rapidly under usual experimental laboratory conditions.

For this study, we used Fourier transform spectra of H_2O_2 recorded at Giessen, Firenze, Denver, and Paris in different spectral ranges (10-430 cm^{-1}, 1250-1370 cm^{-1}, and 370-1270 cm^{-1}) which cover the torsion-rotation band, the ν_6 band, and parts of both bands respectively.

*Line positions: In addition to the vibration-rotation resonances involving the ground state, the ν_3=1, ν_2=1 and ν_6=1 vibrational states, the Hamiltonian model takes explicitly into account both the torsional-rotational resonances within the ground or the ν_6=1 vibrational states, and the "staggering" effect which is due to the tunneling through the cis potential barrier.

*Line intensities: For both spectral regions, the relative intensities for the different torsional sub-bands were deduced from the torsional dependence of the torsion-rotation and ν_6 transition dipole-moment operators.

For the torsion-rotation band (far infrared), the intensities were calibrated in absolute by using the permanent dipole moment measured by Stark effect

For the ν_6 band, the intensities were calibrated in absolute relative to the far infrared region by using Fourier transform spectra recorded in the spectral region covering both the R branch of the torsion-rotation band and the P branch of the ν_6 band.

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SIMULTANEOUS ROVIBRATIONAL ANALYSIS OF THE n_2, n_3, n_5, AND n_6 BANDS OF $H_3{}^{12}CF$ AND $H_3{}^{13}CF$

Dušan Papoušek,
Zlicinska 18, 169 00 Prague 6
CZECH REPUBLIC

Manfred Winnewisser, Stefan Klee,
Physikalisch-Chemisches Institut, Justus-Liebig Universität Giessen
Heinrich-Buff Ring 58, D-35392 Giessen
GERMANY

J. Demaison,
Laboratoire de Spectroscopie Hertzienne, URA CNRS 249, Bât. P5
Université de Lille I, 59655 Villeneuve D'Ascq Cedex
FRANCE

and

Petr Pracna
J. Heyrovsky Institute of Physical Chemistry
Czech Academy of Sciences
Dolejskova 3, 182 23 Prague 8
CZECH REPUBLIC

The four ν_2, ν_3, ν_5, and ν_6, fundamental bands and rotational transitions in the $\nu_2 = 1$, $\nu_3 = 1$, $\nu_5 = 1$, and $\nu_6 = 1$ vibrational states of two isotopomers of methylfluoride ($H_3{}^{12}CF$ and $H_3{}^{13}CF$) were analyzed simultaneously by taking into account various Coriolis interactions, l-type interactions, and alpha-resonance terms between and within these vibrational states. The global treatment of the four-level system leads to a significant improvement of data reproduction providing the standard deviation of 0.76×10^{-4} / 1.16×10^{-4} cm^{-1} for the infrared data of $H_3{}^{12}CF$ / $H_3{}^{13}CF$, respectively, and 150 / 245 kHz for the rotational data.

DEPENDENCE OF MODTRAN ON HITRAN

Alexander Berk
Spectral Sciences, Inc.
99 S. Bedford St., Suite #7
Burlington MA 01803-5169

MODTRAN4, the AFRL atmospheric transmission, radiance and flux model, relies on a statistical band model and the correlated-k method to calculate its radiative transport. The band model depends explicitly and implicitly on the distribution of atmospheric molecular line positions and strengths. HITRAN provides the data required to calculate band model parameters and to validate presumed line distributions. This dependence of MODTRAN on HITRAN will be demonstrated.

FLAASH AND MODTRAN4: STATE-OF-THE-ART ATMOSPHERIC MITIGATION ALGORITHMS FOR HYPERSPECTRAL DATA RETRIEVALS AND SIMULATIONS

Gail P. Anderson, Brian D. Pukall, C. L. Allred, Laila S. Jeong, Michael L. Hoke, and James H. Chetwynd
Air Force Research Laboratory, Space Vehicles Directorate
Hanscom AFB MA 01731

Steven Adler-Golden, Alexander Berk, Larry S. Bernstein, S. Richtsmeier, Prabat K. Acharya, and Michael W. Matthew
Spectral Sciences, Inc.
99 South Bedford St.
Burlington MA 01803

FLAASH (Fast Line-of-sight Atmospheric Analysis of Spectral Hypercubes) is a MODTRAN4-based "atmospheric mitigation" algorithm which is being developed by the Air Force Research Laboratory, Hanscom AFB and Spectral Sciences, Inc. to support current and planned IR-visible-UV hyperspectral and multispectral sensor measurements, typically in image format. The AF intent is to provide surface reflectance and emissivity image cubes of sufficient accuracy for input into surveillance and detection analyses. The atmosphere is effectively removed from the hypercubes, leaving only the spectral signatures of the surface features.

The main objectives are: (1) accurate, physics-based derivation of surface and atmospheric properties (such as surface albedo and emissivity, relative surface altitude, water vapor column, aerosol and cloud optical depths, surface and atmospheric temperatures), (2) minimal computation time requirements, and (3) an interactive, user-friendly interface for generating MODTRAN4-based look-up tables. FLAASH is written in the Interactive Data Language (IDL) for compatibility with a wide variety of computer platforms and to facilitate its use with IDL-based display/analysis software such as ENVI.

Current validation exercises are being carried out on AVIRIS and HYDICE, with applications planned for infrared sensors like ARES/SEBASS. The algorithm for deriving the surface and atmospheric properties utilizes the full MODTRAN4 accuracy (thermal and solar) and accounts for adjacency effects associated with atmospheric scattering. Compared to previous versions of MODTRAN, the new correlated-k radiation transport algorithm provides improved accuracy in treating scattering, especially under conditions of partial cloud and/or aerosol contamination.

FTIR REMOTE SENSING OF ATMOSPHERIC COMPOUNDS: APPLICATION TO GLOBAL CHANGE

Gabriel J. Vazquez
Instituto de Física, UNAM
AP-48-3, Av. Universidad s/n, Col Chamilpa
Cuernavaca, Morelos 62251
MEXICO
(permanent address)

and
National Center for Atmospheric Research
Atmospheric Chemistry Division, P.O. Box 3000
Boulder CO 80307

In this contribution I first underline the need and relevance of measuring gas-phase atmospheric compounds. This point will be illustrated in the context of outstanding environmental issues of current concern such as the greenhouse effect, the ozone-hole in Antartica, the increasing levels of UV radiation at ground level and urban air pollution.

I then describe an application of Fourier Transform Infrared Spectroscopy to the monitoring of atmospheric compounds, namely, Solar Absorption Spectroscopy. I first present an overview of the technique and discuss its use as a tool to determine atmospheric composition. I then report FTIR solar spectroscopy measurements carried out at ground level at NCAR employing a spectrometer of 0.06-cm^{-1} resolution. Sample atmospheric spectra and fitting examples are presented for key species relevant to stratospheric chemistry and global change: ozone (O_3), a chlorofluorocarbon (CF_2Cl_2), a greenhouse gas (N_2O), HCl, NO, and HNO_3.

Solar spectroscopy measurements carried out on a regular basis provide long-term trends of key species relevant to global change, e.g., the increase in greenhouse gases and CFC's or the decrease in stratospheric ozone.

I would like to thank Drs. W. Mankin (NCAR) and D. Murcray and D. Stedman (U. of Denver) for the opportunity to become involved in their research work

SOME PROBLEMS IN SPECTROSCOPIC DATA ENCOUNTERED BY THE ILAS DATA PROCESSING

Tatsuya Yokota, Hideaki Nakajima, Makoto Suzuki, and Yasuhiro Sasano
National Institute for Environmental Studies
16-2 Onogawa, Tsukuba Ibaraki 305-0053
JAPAN

The Improved Limb Atmospheric Spectrometer (ILAS) aboard ADEOS measured profiles of chemical species in high latitudinal ozone layer about eight months from November 1996 to the end of June 1997.

Vertical profiles of aerosol extinction coefficient (780 nm), O_3, CH_4, N_2O, HNO_3, H_2O, NO_2 were obtained from the ILAS data. Profiles of pressure, temperature, CFC-11, and CFC-12 have been trying to be retrieved from the ILAS data, but they are still under study to be improved and validated.

We are using HITRAN96 data for the ILAS data retrieval. There are some problems concerning with spectroscopic data which were found in the ILAS data processing.

Accuracy of O_2-A-band line parameter, and reliability and spectral full coverage (753 - 784 nanometers) of temperature dependency on ozone Wulf band cross-section data are necessary for the precise pressure and temperature retrieval.

Spectral feature of aerosols and its contribution in the absorption spectra in the IR region (6.2 - 11.8 micrometers) are important for the retrieval of O_3, CH_4, N_2O, HNO_3, H_2O, NO_2, CFC-11, and CFC-12 profiles. Refractive index data of sulfuric acid type aerosols and PSCs (Polar Stratospheric Clouds), and weight percentage of the PSC composition are necessary to be studied and implemented.

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