



**19-21 JUNE 2000**

**HARVARD-SMITHSONIAN CENTER FOR ASTROPHYSICS  
CAMBRIDGE MA  
USA**



**K. Narahari Rao, 1921-2000**



**Josef Pliva, 1924-2000**

# THE 6<sup>TH</sup> BIENNIAL HITRAN DATABASE CONFERENCE

**19-21 June 2000**  
**Phillips Auditorium**  
**Harvard-Smithsonian Center for Astrophysics**  
**Cambridge MA**

*Monday, 19 June*

- 8:30 Registration  
9:00 Welcoming Address.....Irwin Shapiro, Director  
Harvard-Smithsonian Center for Astrophysics  
9:20 Memorial.....Jon Hougen

## **SESSION 1: SPECTROSCOPY AND DATABASE**

Chair: Kelly Chance

- 9:30 HITRAN2000 .....Laurence Rothman  
10:00 Molecular Spectroscopy.....Jean-Marie Flaud  
10:30 *Break*  
11:00 Diffuse Interstellar Bands .....Michael McCarthy  
11:30 GEISA.....Nicole Jacquinet-Husson

Noon *Lunch*

## **SESSION 2: CROSS-SECTIONS AND SPECTROSCOPIC REQUIREMENTS**

Chair: William Parkinson

- 2:00 UV Cross-sections .....Johannes Orphal  
2:30 Visible Cross-section .....Michel Carleer  
3:00 Spectroscopic Requirements.....Norbert Glatthor

## **POSTER SESSION 1: DATABASE AND REMOTE-SENSING ISSUES**

Chair: Ken Jucks

3:30 – 5:30

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*(continued)*

*Tuesday, 20 June*

**SESSION 3: SPECTROSCOPIC PARAMETERS**

Chair: Curtis Rinsland

- 9:00 Rotational Spectroscopy .....Edward Cohen  
9:30 IR Ozone .....Georg Wagner  
10:00 IR Formaldehyde .....Agnès Perrin  
10:30 *Break*  
11:00 IR Carbon Dioxide and Oxygen .....Laurence Rothman  
11:30 IR Methane.....D. Chris Benner  
Noon *Lunch*

**SESSION 4: SPECTROSCOPIC PARAMETERS**

Chair: Kouichi Yoshino

- 2:00 IR Ammonia.....Isabelle Kleiner  
2:30 IR Methanol .....Li-Hong Xu

**POSTER SESSION 2: NEW SPECTROSCOPIC PARAMETERS**

Chair: David Johnson

3:00 – 5:00

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*Wednesday, 21 June*

**SESSION 5: WATER VAPOR**

Chair: Laurence Rothman

- 9:00 Theory .....Laurent Coudert  
9:20 Thermal Infrared .....David Steyert  
9:40 Assignments in the Visible Region.....Lawrence Giver  
10:00 Care and Feeding of Databases.....James Brault  
10:20 Self- and Air-Broadening.....Prasad Varanasi  
10:40 *Break*  
11:00 New Parameters for 0.94- $\mu\text{m}$  Region .....Linda Brown  
11:20 Weak Lines in the Near-IR and Visible.....Roland Schermaul  
11:40 New Studies in the Near-IR and Visible.....Djedjiga Belmiloud

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*End of Meeting*

## TABLE OF CONTENTS

### SESSION 1: SPECTROSCOPY AND DATABASE

|  |   |
|--|---|
| HITRAN2000<br>Laurence S. Rothman.....   | 1 |
| MOLECULAR SPECTROSCOPY: A CRUCIAL TOOL FOR ATMOSPHERIC REMOTE<br>SENSING<br>Jean-Marie Flaud .....   | 2 |
| IN PURSUIT OF THE CARRIERS OF THE DIFFUSE INTERSTELLAR BANDS<br>Michael C. McCarthy and Patrick Thaddeus .....                                     | 3 |
| THE CURRENT GEISA SPECTROSCOPIC DATABASE SYSTEM AND ITS EVOLUTION<br>Nicole Jacquinet-Husson, Noëlle Scott, Alain Chédin, and Alexei Chursin ..... | 4 |

### SESSION 2: CROSS-SECTIONS AND SPECTROSCOPIC REQUIREMENTS

|  |   |
|--|---|
| UV-VISIBLE ABSORPTION CROSS-SECTIONS OF ATMOSPHERIC MOLECULES AND<br>RADICALS IN SUPPORT OF GOME AND SCIAMACHY<br>Johannes Orphal, Konstanze Bogumil, Oliver C. Fleischmann, Heike Kromminga, Peter Spietz,<br>Susanne Voigt, and John P. Burrows.....                     | 6 |
| HIGH-RESOLUTION MEASUREMENTS OF THE NO <sub>2</sub> VISIBLE ABSORPTION CROSS-<br>SECTION: TEMPERATURE AND PRESSURE EFFECTS<br>Ann-Carine Vandaele, Christian Hermans, Sophie Fally, Michel R. Carleer, Reginald Colin,<br>Marie-France Mérienne, and Alain Jenouvrier..... | 7 |
| SPECTROSCOPIC REQUIREMENTS FOR MIPAS/ENVISAT ANALYSIS OF PROCESSES<br>RELATED TO THE UPPER TROPOSPHERE AND LOWER STRATOSPHERE<br>Gabriele P. Stiller, Norbert Glatthor, and Sylvia Kellmann .....  | 8 |

### POSTER SESSION 1: DATABASE AND REMOTE-SENSING ISSUES

|  |    |
|--|----|
| P1. JAVAHAWKS: THE SOFTWARE SYSTEM FOR ACCESSING AND FILTERING THE<br>HITRAN DATABASE<br>John Schroeder and Laurence S. Rothman .....  | 9  |
| P2. A WEB INTERFACE FOR THE HITRAN DATABASE<br>Eliot F. Young and Sky Coyote .....   | 10 |
| P3. EINSTEIN A COEFFICIENT, INTEGRATED BAND INTENSITY, AND POPULATION<br>FACTORS. APPLICATION TO THE $A^1\Delta_g - X^3\Sigma_g^-(0,0)$ O <sub>2</sub> BAND<br>Robert R. Gamache and Aaron Goldman ..... | 11 |
| P4. INDICES OF REFRACTION FOR HITRAN 2000<br>Steven T. Massie and Aaron Goldman .....  | 12 |
| P5. CONTINUUM ABSORPTION BY ATMOSPHERIC GASES<br>Belén Maté, Catherine L. Lugez, Alexander M. Solodov, Gerald T. Fraser, and Walter J. Lafferty  | 13 |

|   |    |
|---|----|
| P6. COLLISION-INDUCED ABSORPTION IN N <sub>2</sub> -H <sub>2</sub> O: APPLICATION OF HITRAN DATABASE  |    |
| Alexander Brown and Richard H. Tipping .....  | 14 |
| P7. THE DENSITY MATRIX OF H <sub>2</sub> O-H <sub>2</sub> O IN THE COORDINATE REPRESENTATION: A MONTE CARLO CALCULATION OF THE FAR-WING LINE SHAPE            |    |
| Qiancheng Ma and Richard H. Tipping .....   | 15 |
| P8. RECENT AND REQUIRED UPDATES IN FAR-INFRARED SPECTROSCOPY FOR PRECISE ATMOSPHERIC OBSERVATIONS   |    |
| Kenneth W. Jucks, David G. Johnson, Wesley A. Traub, and Kelly V. Chance.....   | 16 |
| P9. REMOTE-SENSED FORMALDEHYDE OBSERVATIONS FROM THE ESA GOME INSTRUMENT  |    |
| Kelly Chance, Paul I. Palmer, Randall V. Martin, Robert J. D. Spurr, Thomas P. Kurosu, and Daniel J. Jacob .....  | 17 |
| P10. COMPARISON OF SPECTRAL AND GEOMETRIC METHODS FOR RETRIEVING CLOUD PARAMETERS FROM DOWNWELLING FTIR SPECTRA IN THE ARCTIC                                 |    |
| Steven Neshyba.....   | 18 |
| P11. POLAR STRATOSPHERIC CLOUD DETECTION FROM THE ILAS INSTRUMENT   |    |
| Thomas P. Kurosu, Tatsuya Yokota, Kelly Chance, and Yasuhiro Sasano.....  | 19 |
| P12. ANALYSIS OF THE ILAS LIMB TRANSMISSION SPECTRA AT 753 - 784 nm: COMPARISONS ON O <sub>2</sub> -A-BAND LINE PARAMETERS AND OZONE WULF BAND CROSS-SECTIONS |    |
| Tatsuya Yokota, Takafumi Sugita, Hideaki Nakajima, and Yasuhiro Sasano .....  | 20 |
| P13. HITRAN CONSIDERATIONS FOR HIRDLS   |    |
| David P. Edwards, Steve Massie, John C. Gille, Aaron Goldman, and John Ballard .....  | 21 |
| P14. THE ISSWG LINE-BY-LINE INTERCOMPARISON   |    |
| Stephen A. Tjemkes .....  | 22 |
| P15. SPECTROSCOPIC REQUIREMENTS FOR MIPAS/ENVISAT NON-LTE ANALYSIS  |    |
| Bernd Funke, Francisco J. Martin-Torres, Gabriele P. Stiller, Manuel Lopez-Puertas, and Norbert Glatthor .....  | 23 |
| P16. REQUIREMENT FOR REFRACTIVE INDICES FOR MIPAS/ENVISAT PSC ANALYSIS  |    |
| Alexandra Zimmermann and Michael Höpfner .....  | 24 |
| P17. THE NEED FOR WATER AND METHANE SPECTROSCOPIC DATA FOR THE INTERPRETATION OF SCIAMACHY NEAR-INFRARED MEASUREMENTS   |    |
| Hans Schrijver.....   | 25 |
| P18. LIDAR EQUATION MODELING USING LIDAR-PC AND THE HITRAN DATABASE   |    |
| Dennis K. Killinger.....  | 26 |

### SESSION 3: SPECTROSCOPIC PARAMETERS

#### ROTATIONAL SPECTROSCOPY IN SUPPORT OF UPPER ATMOSPHERIC RESEARCH AT JPL

Edward A. Cohen, Brian J. Drouin, Charles E. Miller, and Holger S.P. Müller ..... 27

#### A NEW SPECTROSCOPIC DATABASE FOR THE OZONE FUNDAMENTALS

Georg Wagner, Manfred Birk, Franz Schreier, and Jean-Marie Flaud..... 28

#### HIGH-RESOLUTION ANALYSIS OF H<sub>2</sub>CO IN THE 3.6- AND 4.3-MICROMETER REGIONS

Agnès Perrin, Jean-Marie Flaud, Phillip Arcas, Alain Valentin, and Claude Camy-Peyret..... 29

#### THE VENUS 1- $\mu$ m CO<sub>2</sub> BANDS AND THE O<sub>2</sub> (0-1) $X^3\Sigma_g^- - A^1\Delta_g$ AND (1-0) $X^3\Sigma_g^- - B^1\Sigma_g^+$ BANDS IN THE EARTH'S ATMOSPHERE

Aaron Goldman, Thomas M. Stephen, Laurence S. Rothman, Lawrence P. Giver, Jean-Yves Mandin, Robert R. Gamache, Curtis P. Rinsland, and Frank J. Murcray..... 30

#### CHARACTERIZATION OF THE $\nu_3$ BAND OF METHANE

D. Chris Benner, V. Malathy Devi, and Mary Ann H. Smith..... 31

### SESSION 4: SPECTROSCOPIC PARAMETERS

#### INFRARED SPECTROSCOPY OF AMMONIA $^{14}\text{NH}_3$

Isabelle Kleiner ..... 32

#### BENCHMARK LABORATORY METHANOL DATA AT THE UNIVERSITY OF NEW BRUNSWICK, CANADA

Li-Hong Xu and Ronald M. Lees ..... 33

### POSTER SESSION 2: NEW SPECTROSCOPIC PARAMETERS

#### P19. SOME NEW LABORATORY MEASUREMENTS AND THEIR EFFECT UPON THE SPECTROSCOPIC DATABASE

Prasad Varanasi..... 35

#### P20. METHANE LINE PARAMETERS IN THE MOPITT CHANNELS NEAR 2.3 $\mu$ m (2300 nm)

Adriana Predoi-Cross, Linda R. Brown, Robert A Toth, V.Malathy Devi, and D.Chris Benner... 36

#### P21. AIR-, N<sub>2</sub>- AND SELF-BROADENING AND SHIFT COEFFICIENTS AND LINE MIXING IN THE $\nu_3$ , $\nu_5$ AND $\nu_6$ BANDS OF $^{12}\text{CH}_3\text{D}$

Mary Ann. H. Smith, V.Malathy Devi, D.Chris Benner, Linda R. Brown, and Robert L. Sams... 37

#### P22. RECENT PROGRESS ACHIEVED IN THE 6.2- $\mu$ m REGION FOR NITROGEN DIOXIDE

Agnès Perrin, Johannes Orphal, Jean-Marie Flaud, Stefan Himmelmann, Susanne Voigt, John P. Burrows, Thomas M. Stephen, Aaron Goldman, and Curtis P. Rinsland..... 38

#### P23. POSITIONS AND INTENSITIES OF AMMONIA HOT BANDS IN THE 4- TO 8- $\mu$ m REGION

Claire Cottaz, Isabelle Kleiner, Ginette Tarrago, and Linda R. Brown..... 40

|   |    |
|---|----|
| P24. HBr AND HI LINE PARAMETERS UPDATE FOR ATMOSPHERIC SPECTROSCOPY DATABASES<br>Aaron Goldman, Michael T. Coffey, James W. Hannigan, William G. Mankin, Kelly V. Chance, and Curtis P. Rinsland .....  | 41 |
| P25. UPDATED ELECTRIC DIPOLE-MOMENT FUNCTION FOR THE GROUND ELECTRONIC STATE OF CARBON MONOXIDE<br>Charles Chackerian, Jr., Richard Freedman, Lawrence P. Giver, Linda R. Brown, and James W. Brault.....   | 42 |
| P26. A MULTISPECTRUM FITTING PROCEDURE TO IMPROVE THE ACCURACY OF LINE PARAMETERS APPLICATION TO THE SECOND OVERTONE OF CO: PRELIMINARY RESULTS<br>Victor Dana, David Jacquemart, Jean-Yves Mandin, Nathalie Picqué, and Guy Guelachvili .....  | 43 |
| P27. REVISITED LINE INTENSITIES OF ACETYLENE $^{12}\text{C}_2\text{H}_2$ IN THE 13.6- $\mu\text{m}$ SPECTRAL REGION<br>David Jacquemart, Victor Dana, Jean-Yves Mandin, and Christophe Claveau .....  | 44 |
| P28. INTENSITY AND LINEWIDTH MEASUREMENTS IN THE 13.7- $\mu\text{m}$ BANDS OF $\text{C}_2\text{H}_2$ AT PLANETARY TEMPERATURES<br>Chengbo Sun, Qunjun Zou, and Prasad Varanasi.....   | 45 |
| P29. ABSOLUTE LINE-INTENSITY MEASUREMENTS IN THE $\nu_2$ BAND OF HOCl<br>Jean Vander Auwera, Joerg Kleffmann, Jean-Marie Flaud, Gottfried Pawelke, and Hans Burger  | 46 |
| P30. A NEW SPECTROSCOPIC DATABASE FOR CHLORINE NITRATE<br>Manfred Birk and Georg Wagner .....   | 47 |
| P31. ABSOLUTE ABSORPTION CROSS-SECTION MEASUREMENTS OF THE SCHUMANN-RUNGE CONTINUUM OF $\text{O}_2$ AT 78K AND 295K<br>Kouichi Yoshino, James R. Esmond, William H. Parkinson, Kenji Ito, and Takashi Matsui.....   | 48 |
| P32. THE APPLICATION OF A VUV FOURIER-TRANSFORM SPECTROMETER AND SYNCHROTRON RADIATION SOURCE TO MEASUREMENTS OF THE $\beta(6,0)$ AND $\gamma(3,0)$ BANDS OF NO<br>Allan S-C. Cheung, D. H-Y. Lo, Karina W-S. Leung, Kouichi Yoshino, James R. Esmond, William H. Parkinson, Anne P. Thorne, Jonathan E. Murray, Richard C.M. Learner, Geoff Cox, Kenji Ito, Takashi Matsui, and Takashi Imajo..... | 49 |
| P33. PREDICTED PREDISSOCIATION LINEWIDTHS IN THE SCHUMANN-RUNGE BANDS OF $\text{O}_2$ COMPARED WITH RECENT HIGH-RESOLUTION MEASUREMENTS<br>G.S-M. Tong, Allan S-C. Cheung, and Michael J. Jamieson .....  | 50 |
| P34. THE ELECTRONIC STRUCTURE OF $\text{NO}_2^+$ . AN AB-INITIO MRD-CI STUDY<br>Gabriel J. Vázquez and Carolina Godoy.....  | 51 |

**SESSION 5: WATER VAPOR**

**IS THE WATER MOLECULE SPECTROSCOPICALLY WELL UNDERSTOOD NOW?**

Laurent H. Coudert ..... 52

**LINE PARAMETERS FOR WATER IN THE THERMAL INFRARED**

David W. Steyert, Weifeng Wang, Neil M. Donahue, J.Marcos Sirota, and Dennis C. Reuter ..... 53

**CONSENSUS ASSIGNMENTS FOR WATER-VAPOR LINES NOT ASSIGNED IN HITRAN  
13,200 TO 16,500 cm<sup>-1</sup>**

Lawrence P. Giver, David W. Schwenke, Charles Chackerian, Jr, Richard S. Freedman, and Prasad Varanasi..... 54

**THE CARE AND FEEDING OF DATABASES**

James W. Brault ..... 55

**EXPERIMENTAL STUDY OF SELF- AND AIR-BROADENED WATER VAPOR LINES**

Qunjun Zou, Prasad Varanasi, and Chengbo Sun..... 56

**LABORATORY SPECTROSCOPY TO SUPPORT EOS: WATER LINE PARAMETERS  
NEAR 0.94 μm (940 nm) FOR SAGE III**

Linda R. Brown and Robert A. Toth..... 57

**WEAK LINES IN THE WATER VAPOUR NEAR-INFRARED AND VISIBLE SPECTRUM**

Roland Schermaul, Antonio A.D. Canas, Richard C.M. Learner, James W. Brault, Djedjiga Belmiloud, Oleg L. Polyansky, and Jonathan Tennyson ..... 58

**NEW STUDIES OF THE VISIBLE AND NEAR-INFRARED ABSORPTION BY WATER  
VAPOUR AND SOME PROBLEMS WITH HITRAN**

Djedjiga Belmiloud, Roland Schermaul, Kevin Smith, Nikolai F. Zobov, James W. Brault, Richard C.M. Learner,<sup>b</sup> David A. Newnham, and Jonathan Tennyson ..... 59

**AUTHOR INDEX**.....60



## HITRAN2000

**Laurence S. Rothman**

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The HITRAN database project has its origins in compilations of spectral parameters for water vapor and carbon dioxide almost four decades ago<sup>1</sup> and culminated in the first public, machine-readable edition<sup>2</sup> in 1973. HITRAN has evolved from a compilation of parameters for the principal atmospheric absorbers in the infrared to a large database covering the microwave through ultraviolet regions, containing additional parameters for the demands of remote-sensing satellite experiments, and with many molecular constituents. A number of papers in this conference demonstrate the more sophisticated high-resolution requirements of remote-sensing experiments sponsored by the US National Aeronautical and Space Agency (NASA), the European Space Agency (ESA), and the National Space Development Agency of Japan. Meanwhile, there has also been great progress in the acquisition of spectral parameters for trace gases, major improvements for the major gases such as water vapor and ozone, and the measurement of cross-section data for the “heavy” gases.

In this presentation, we discuss the features of the next edition of HITRAN which attempt to address many of these problems. A new format for the line-by-line portion of the database and an increased file structure will be shown. There will be a great increase in cross-section data sets, as well as additional data for indices of refraction and UV data. Other related issues are collision-induced absorption data, documentation, and linked tables of data and references.

The complexity of HITRAN in this new millennium, and the limitation of available resources, require an international collaborative effort for this project to succeed. Progress has been made by setting up teams for critical evaluation of data, and the internet and generally available software is providing more rapid dissemination and access of results.

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This effort is being supported by the NASA Earth Observing System (EOS), Grant NAG5-8420 and the Atmospheric Radiation Measurement (ARM) program of the US Department of Energy.

1. D.M. Gates, R.F. Calfee, D.W. Hansen, and W.S. Benedict, “Line Parameters and Computed Spectra for Water Vapor Bands at 2.7 $\mu$ ,” NBS monograph 71 (1964); R.F. Calfee and W.S. Benedict, “Carbon Dioxide spectral line Positions and Intensities Calculated for the 2.05 and 2.7 Micron Regions,” NBS Technical note 332 (1966).
2. R.A. McClatchey, W.S. Benedict, S.A. Clough, D.E. Burch, K. Fox, L.S. Rothman, and J.S. Garing, “AFCRL Atmospheric Absorption Line Parameters Compilation, AFCRL Technical Report 0096 (1973).

## **Molecular Spectroscopy: a Crucial Tool for Atmospheric Remote Sensing**

**Jean-Marie Flaud**

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Passive remote sensing techniques are widely used to probe the terrestrial atmosphere and retrieve P,T profiles as well as concentration profiles of a number of minor atmospheric constituents. Nowadays the techniques which are used (Fourier transform interferometers, diode laser spectrometers,...) are more and more sophisticated (better resolution, better signal-to-noise ratio, coverage of large spectra domains,...). This implies a huge effort to generate the accurate spectroscopic parameters (both for the species of interest and for the interfering species) which are needed for reliable retrievals of atmospheric profiles. To illustrate this point some examples will be given.

First it will be shown that for the ClONO<sub>2</sub> molecule, despite recent high-resolution studies, the situation is not yet completely satisfactory and that more spectroscopic work is needed in order to meet the atmospheric needs.

Then recent spectroscopic studies undertaken in order to generate spectral parameters involving the highly excited vibrational states of the ozone molecule will be described as well as their use in the modeling of non-LTE (non local thermodynamic equilibrium) phenomena in the atmosphere and the application to the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment.

Finally, if time permits, recent results concerning the spectroscopy of HOCl and O<sub>3</sub> will be concisely discussed.

## In Pursuit of the Carriers of the Diffuse Interstellar Bands

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One of the outstanding unsolved problems in astronomical spectroscopy is the origin of the diffuse interstellar bands. The carriers may be crucially important in interstellar chemistry: they may constitute a significant fraction of all chemically-bonding matter in the interstellar gas, and many may be molecules larger than any so far identified in space with radio telescopes. The carriers are widely believed to be gas-phase molecules, and long carbon chains and rings are some of the best candidates. Although additional theory and astronomical observations are needed, the identity of the carriers is now essentially a problem in laboratory astrophysics, and recent advances in our laboratory and others have demonstrated that the means are now at hand to tackle this important problem. Detection has proved challenging, but more than 75 new carbon molecules have now been detected over the past three years by means of Fourier-transform microwave and laser cavity ringdown absorption spectroscopies in supersonic molecular beams. Four of these new molecules are hydrocarbon chains that are nonpolar by symmetry, but which possess strong electronic spectra in the visible. By the same technique, a fairly strong molecular absorption band closely centered on the strongest and best known diffuse band at 4428.9 Angstroms has recently been found among the products of a discharge through benzene and other hydrocarbons. We have not yet been able to determine the exact elemental formula or structure of the carrier of the laboratory band, nor have we been able to demonstrate with certainty that the laboratory band is the same as that observed in space, but the agreement in wavelength between the two is so good (a few parts in 10,000) that a chance coincidence would seem unlikely.

## The Current Geisa Spectroscopic Database System and its Evolution

Nicole Jacquinet-Husson,<sup>a</sup> Noëlle Scott,<sup>a</sup> Alain Chédin,<sup>a</sup> and Alexei Chursin<sup>b</sup>

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*Tomsk*

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Accurate spectral analyses of Earth or planetary spectra observed by new generations of high spectral resolution vertical atmospheric sounders will result in an improved knowledge of their atmospheric and surface properties. The performance of instruments like AIRS (Atmospheric Infrared Sounder) in the USA, and IASI (Infrared Atmospheric Sounding Interferometer) in Europe, which have a better vertical resolution and accuracy, compared to the presently existing satellite infrared temperature sounders, is directly related to the quality of the spectroscopic parameters of the optically active gases, since these are essential input in the forward models used to simulate recorded radiance spectra. In this context, the ARA (Atmospheric Radiation Analysis) group at LMD (Laboratoire de Météorologie Dynamique, France) has developed the GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information) computer-accessible database system, since 1974. This early effort implemented the so-called « line-by-line and layer-by-layer » approach for forward radiative transfer modelling action. This activity is of interest to research groups dealing with direct and inverse radiative transfer studies. Currently, GEISA is involved in activities, with the purpose of assessing the IASI measurements capabilities and its own database quality, within the ISSWG (IASI Sounding Science Working Group), in the frame of the CNES (Centre National d'Etudes Spatiales, France)/EUMETSAT (European organization for the exploitation of METeorological SATellites) Polar System (EPS), by simulating high-resolution radiances and/or using experimental data.

The contents, as well as the access and management facilities, of the last 1997 public version1 of the Internet-accessible GEISA spectroscopic database system, will be presented. The individual line description of GEISA-97 contains 1,336,266 entries belonging to 42 molecules (96 isotopic species) and located between 0 and 22,656  $\text{cm}^{-1}$ . It has molecules of interest for both terrestrial and other planetary atmospheres, especially those of the Giant Planets. GEISA-97 also has a catalog of absorption cross-sections of molecules such as chlorofluorocarbons with complex spectra that are too dense for direct parameterization. Illustrations of the Web facilities of the GEISA system will be given.

For the upcoming high spectral resolution atmospheric sounders, the so-called GEISA/IASI sub-database system has been elaborated, from GEISA-97. Its content, which will be the spectroscopic parameters reference for IASI direct radiative transfer modelling, with enhanced or new cross-sections and specific aerosol data as well, will be described.

The IASI soundings spectroscopy requirements, previously emphasized,<sup>2</sup> will be discussed in the context of comparisons between recorded and calculated experimental spectra. Subsequent consolidated versions of GEISA and GEISA/IASI will be presented. This work is ongoing in the frame of ISSWG projects supported by CNES (GEISA/IASI project) and by the

European Commission Environment and Climate Programme (VIRTEM-Validation of IASI Radiative Transfer: Experiments and Modelling- project).

1. N. Jacquinet-Husson et al (48 co-authors), *J. Quant. Spectrosc. Radiat. Transfer* **62**, 205 (1999).
2. N. Jacquinet-Husson, N.A. Scott, A Chédin, B. Bonnet, A. Barbe, Vl.G. Tyuterev, J.P. Champion, M. Winnewisser, L.R. Brown, R. Gamache, V.F. Golovko and A.A. Chursin, *J. Quant. Spectrosc. Radiat. Transfer* **59**, 511 (1998).

## UV-visible Absorption Cross-sections of Atmospheric Molecules and Radicals in Support of GOME and SCIAMACHY

Johannes Orphal,<sup>a</sup> Konstanze Bogumil,<sup>b</sup> Oliver C. Fleischmann,<sup>b</sup> Heike Kromminga,<sup>b</sup>  
Peter Spietz,<sup>b</sup> Susanne Voigt,<sup>b</sup> and John P. Burrows<sup>b</sup>

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In recent years, we have measured temperature dependent UV-visible absorption cross-sections of the atmospheric molecules and radicals O<sub>3</sub>, NO<sub>2</sub>, OCIO, and BrO in support of the GOME (Global Ozone Monitoring Experiment) and SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartography) satellite projects, using different techniques: multichannel diode-array grating spectrometers (GOME-FM and SCIAMACHY-FM), high-resolution Fourier-transform spectroscopy (Bruker IFS-120-HR), and time-resolved flash-photolysis spectroscopy. In this paper, the results are compared with previously published data, and recommendations for remote-sensing applications are made.

**High-resolution Measurements of the NO<sub>2</sub> Visible Absorption  
Cross-section: Temperature and Pressure Effects**

**Ann-Carine Vandaele,<sup>a</sup> Christian Hermans,<sup>a</sup> Sophie Fally,<sup>b</sup> Michel R. Carleer,<sup>b</sup>  
Reginald Colin,<sup>b</sup> Marie-France Mérienne,<sup>c</sup> and Alain Jenouvrier<sup>c</sup>**

*<sup>a</sup>Belgian Institute for Space Aeronomy*

*<sup>b</sup>Laboratoire de Chimie Physique Moléculaire, University of Brussels  
BELGIUM*

*<sup>c</sup>GSMA, University of Reims  
Reims  
FRANCE*

The absorption cross-section of NO<sub>2</sub> has been investigated at high resolution (0.05 and 0.1 cm<sup>-1</sup>) in the visible region (11000 - 22300 cm<sup>-1</sup>). Measurements have been performed under various conditions of pressure (pure NO<sub>2</sub>, NO<sub>2</sub> diluted in a mixture of N<sub>2</sub>+O<sub>2</sub> with dilutions of 9.6 ppm, 92 ppm, and 965 ppm), and at three temperatures (293K, 240K, and 220K). This paper will show preliminary results on the effects of the temperature and of the pressure on the absorption cross-section of NO<sub>2</sub>. It is now widely admitted that the temperature effect must be taken into account when performing stratospheric detection of NO<sub>2</sub>. It will also be shown that cross-sections obtained under conditions close to the atmospheric ones must be used in order to account for a pressure effect.

## **Spectroscopic Requirements for MIPAS/ENVISAT Analysis of Processes Related to the Upper Troposphere and Lower Stratosphere**

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MIPAS (Michelson Interferometer for Passive Atmospheric Soundings) on ENVISAT will offer the opportunity to study atmospheric processes in the upper troposphere (UT) and lower stratosphere (LS). For a number of trace species detection would be most favorable for the understanding of chemical and dynamical processes. However, spectroscopic information in the MIPAS spectral channels is lacking completely, or is available with insufficient accuracy only. In the UT, examples for these species are formaldehyde ( $\text{H}_2\text{CO}$ ), acetone ( $\text{CH}_3\text{COCH}_3$ ), and peroxy acetyl nitrate (PAN,  $\text{CH}_3\text{CO}_3\text{NO}_2$ ). All these substances are involved in the chemical processing of ozone which is not yet completely understood. In the LS the observation of a number of halogenated species like bromo-methane ( $\text{CH}_3\text{Br}$ ) or methyl chloroform ( $\text{CH}_3\text{CCl}_3$ ) would benefit from spectroscopic data being made or being improved. On the basis of absorption cross-sections derived from low-resolution absorption spectra that are commercially available, we shall demonstrate the significance of the signatures of these species in simulated MIPAS spectra and estimate accuracy and other requirements for spectroscopic data.

## **P1. JavaHAWKS: the Software System for Accessing and Filtering the HITRAN Database**

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The software system being developed for the next edition of HITRAN is being written in the JAVA programming language. This language was chosen over the previous language for HAWKS (HITRAN Atmospheric Workstation) due to considerations of cross-platform application. The goal was to write the same code that would work on PCs, UNIX workstations, and MACs. New features that have already been implemented are improved plotting of the line-by-line portion of the compilation and capabilities of plotting the cross-section data. The most important feature of the previous software, namely the SELECT menu, is still available for the user to filter and manipulate portions of the line-by-line database as well as other databases in HITRAN format. A more “readable” form of the database can also be extracted.

In the future we plan to implement the HAWKS software on the world-wide-web, enhance the plotting capabilities, facilitate non-local thermodynamic equilibrium (non-LTE) applications, and improve high-temperature applications.

## **P2. A Web Interface for the HITRAN Database**

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Under the auspices of the NASA's Applied Information Systems Research Program, we have developed a plug-in for Netscape Web Browsers that allows the user to run local, native applications from an HTML form. We will present an HTML interface to the SELECT programs which are distributed on the HITRAN-96 CD-ROMs.

**P3. Einstein A Coefficient, Integrated Band Intensity, and Population Factors. Application to the  $a^1D_g - X^3S_g^- (0,0)$   $O_2$  Band**

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Literature values of the Einstein A coefficient for spontaneous emission for the  $a^1\Delta_g \rightarrow X^3\Sigma_g^-$  band of  $O_2$  differ by as much as a factor of 2. The corresponding integrated band intensity values found in the literature show maximum differences of a factor of 4. The reason for these differences is not only the spread in the measured absorption band strengths but also in the improper use of population factors relating the Einstein A value to the line intensity or integrated band intensity. Here, the relationship between the Einstein A coefficient for spontaneous emission and the integrated band intensity and line intensity are developed with application to  $a^1\Delta_g \leftarrow X^3\Sigma_g^-$  band of  $O_2$ . Previous work, on these relationships, demonstrate much confusion of the proper use of the lower and upper state population factors with some using a ratio of 3:1 and the others 3:2. A slightly modified expression for the line intensity in terms of the integrated band intensity is proposed which corrects for some approximations used in earlier expressions. Finally suggestions are made for the values of the electronic-vibrational Einstein A coefficient and integrated band intensity for the  $a^1\Delta_g \leftarrow X^3\Sigma_g^-$  band of  $O_2$ .

## **P4. Indices of Refraction for HITRAN 2000**

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The HITRAN 2000 database will include recent measurements of temperature-dependent indices of refraction over a wide wavelength range for several aerosol composition types: H<sub>2</sub>SO<sub>4</sub>/H<sub>2</sub>O, HNO<sub>3</sub>/H<sub>2</sub>O, NAT, NAD, water ice, and the indices of burning vegetation. The data sets are reviewed, and graphs intercompare the new indices and representative aerosol spectra. While the new cold temperature indices of refraction of H<sub>2</sub>SO<sub>4</sub>/H<sub>2</sub>O are an improvement over those measured previously at room temperature, there are noticeable differences between the recent cold-temperature measurements.

## **P5. Continuum Absorption by Atmospheric Gases**

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The continuum induced absorption coefficients for the 1.27-micrometer and the 6.4-micrometer bands of O<sub>2</sub> have been measured using a Fourier-transform infrared spectrometer with an optical path length of 84 m. Spectra were recorded for both pure O<sub>2</sub> and O<sub>2</sub>/N<sub>2</sub> mixtures at densities up to 10 amagats and temperatures between 296 K and 233 K. Also, the intensity of the simultaneous vibrational collision-induced absorption band CO<sub>2</sub>(v=1) + N<sub>2</sub>(v=1) → CO<sub>2</sub>(v=0) + N<sub>2</sub>(v=0) at 4880 cm<sup>-1</sup> has been measured using pressures between 5 and 10 amagats. The absorption coefficients obtained are compared with previous laboratory and atmospheric measurements.

## **P6. Collision-Induced Absorption in N<sub>2</sub>-H<sub>2</sub>O: Application of HITRAN Database**

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We have calculated the collision-induced absorption of N<sub>2</sub>-H<sub>2</sub>O in the spectral region of the N<sub>2</sub> fundamental for a range of atmospheric temperatures. The dominant induction mechanism is the dipole-induced dipole, in which the H<sub>2</sub>O molecule makes a pure-rotational allowed transition whose intensity and position are obtained from the HITRAN database, and the N<sub>2</sub> molecule makes a vibration-rotational Raman transition. Thus, the frequency range of absorption is between 2200 - 2800 cm<sup>-1</sup>. Because this mechanism is much stronger than the quadrupole-induced dipole responsible for the well-known N<sub>2</sub>-N<sub>2</sub> collision-induced absorption, the absorption coefficient per pair is much larger. In the atmosphere, because the number density of H<sub>2</sub>O molecules is much less than that of N<sub>2</sub>, the latter absorption dominates in the lower frequency part of the spectrum. However, for 100% humidity at T = 300K, the two absorptions are equal at approximately 2500 cm<sup>-1</sup>, and at higher frequencies, the N<sub>2</sub>-H<sub>2</sub>O absorption dominates. Because the frequency region beyond the ν<sub>3</sub> band head of CO<sub>2</sub> is widely used to obtain atmospheric retrievals, one has to have an accurate forward model, including not only the effects of line-mixing in CO<sub>2</sub>, but also the self and foreign water continua, and the important collision-induced absorptions. The present results will be compared with some previous measurements and the conclusions discussed.

## **P7. The Density Matrix of H<sub>2</sub>O-H<sub>2</sub>O in the Coordinate Representation: A Monte Carlo Calculation of the Far-Wing Line Shape**

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With the formalism developed previously for the calculation of the far-wing line shape for molecular systems, the complete set in Hilbert space is constructed from the states of the absorber and bath molecules. As a result, one has to spend most of the computer resources to diagonalize the anisotropic potential matrix whose size is determined by the number of states included. For systems of interest in atmospheric applications, this limited the number of states that could be included and the accuracy attainable. Recently, a new formalism has been developed in which the eigenfunctions of the orientations of the system are chosen as the complete set. The advantage of this coordinate representation is that the diagonalization procedure becomes unnecessary and as many states as desired can be included in the calculation of the density matrix which is the only off-diagonal operator. Then, the main computational task is to carry out multidimensional integrations over the continuous variables which specify the initial and final orientations of the systems during transition processes. For the complicated systems of interest consisting of two asymmetric-top molecules, the dimension of integrations is 11. In order to evaluate such high-dimensional integrations, one has to rely on the Monte Carlo method. Meanwhile, we have also developed an interpolation procedure which enables one to consider more sophisticated potentials such that their dependence on  $r$  and on orientation interweave and the dependence on  $r$  takes a complicated form. Combining these two improvements, we are able to calculate converged far-wing line shapes for H<sub>2</sub>O-H<sub>2</sub>O from realistic potential models, e.g., those that yield realistic virial coefficients or transport data. Results will be presented and compared with experiments.

## P8. Recent and Required Updates in Far-Infrared Spectroscopy for Precise Atmospheric Observations

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Far infrared transitions of the isotopomers of H<sub>2</sub>O can be used to retrieve the isotopic fractionation of H<sub>2</sub>O in the stratosphere, which in turn can be used to study the transport processes for air entering the stratosphere. While the isotopic depletion for HDO is large, it is not for H<sub>2</sub><sup>18</sup>O and H<sub>2</sub><sup>17</sup>O compared to the standard lower tropospheric abundances. As a result, the absolute strengths for these transitions, as well as H<sub>2</sub><sup>16</sup>O must be accurate to a few percent or better for statistically meaningful retrievals of the isotopic fractionation. The current HITRAN strengths are insufficient. We have used recent calculations of strengths (from L. Coudert in Paris and John Pearson at JPL) to improve our atmospheric retrievals from the FIRS-2 spectrometer, but more work is required.

Other spectroscopy that needs improvement in the far-IR include the hot and combination bands to the red of the  $\nu_9$  band of HNO<sub>3</sub> at 458 cm<sup>-1</sup>. These bands all fall within 400 and 450 cm<sup>-1</sup> and are quite strong features in atmospheric spectra. They also fall in locations that overlap with broad features that can be used to retrieve ClNO<sub>3</sub> and N<sub>2</sub>O<sub>5</sub> from past spectra in high aerosols when Chlorine and Nitrogen chemistry in the stratosphere were most highly perturbed from volcanic aerosols. These remain open questions in stratospheric chemistry. Improved broadening parameters for the strong H<sub>2</sub>O transitions in this region would also improve the retrievals from these broad features by reducing residuals. Accurate cross-sections are still needed for the broad ClNO<sub>3</sub> feature near 430 cm<sup>-1</sup>.

## **P9. Remote-sensed Formaldehyde Observations from the ESA GOME Instrument**

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Formaldehyde (HCHO) is an important indicator of photochemical activity and hydrocarbon reactivity in the troposphere. We present vertical column abundances of HCHO retrieved from the Global Ozone Monitoring Experiment (GOME) spectrometer aboard the ERS-2 satellite. Previous GOME studies have shown that HCHO can be measured from space. The present study provides the sensitivity to measure HCHO globally for the first time.

We determine slant columns of HCHO to 0.2 DU sensitivity by directly fitting GOME radiances using a nonlinear least-squares algorithm. We transform the slant columns to total vertical columns by correcting for vertical profile variability in the presence of Rayleigh and aerosol scattering. This transformation is achieved using the LIDORT multiple scattering radiative transfer model in conjunction with vertical profile shapes derived from the Harvard-GEOS global 3-D model of tropospheric chemistry. Total HCHO columns over North America in July 1996 are compared with in-situ surface and aircraft measurements and with the Harvard-GEOS model. Selected examples of HCHO from biomass burning in South America, Asia, and Africa are also presented.

**P10. Comparison of Spectral and Geometric Methods  
for Retrieving Cloud Parameters  
from Downwelling FTIR Spectra in the Arctic**

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We present a comparison of two methods for retrieving cloud parameters from downwelling infrared spectra taken in the Arctic during March/April 1998, as part of the Surface Heat Budget of the Arctic project SHEBA. Both methods employ an isothermal cloud model that incorporates the effects of Mie scattering of liquid and ice particles. One method in the comparison the spectral method relies on the frequency dependence of optical depth in the 8-12 micrometer region due to the cloud, combined with a clear-sky model extracted from MODTRAN. Temperature profiles for the radiative transfer calculation are provided by radiosondes from the SHEBA project office. Retrieved cloud parameters are temperature, ice/liquid water fraction, condensed water path, and cloud particle size. The latter three may be combined into an optical depth spectrum. The second method in the comparison, the geometric method, is based entirely on the geometric dependence of optical depth in selected microwindows of the same spectral range. Retrieved cloud parameters are temperature and optical depth. Self-consistency of the spectral method itself is evaluated by comparing results at different viewing angles. The mutual consistency of the two methods is evaluated by comparing optical depths. We also present an analysis of the statistical significance of multi-parameter retrievals in the presence of instrument noise and cloud horizontal inhomogeneity.

## **P11. Polar Stratospheric Cloud Detection from the ILAS Instrument**

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Polar stratospheric clouds (PSCs) play an important role in stratospheric ozone depletion due to denitrification of the atmosphere which is associated with their formation and the resulting enhancement in halogen free-radical chemistry. We present a fast and simple method for PSC detection from observations of the Environment Agency of Japan's Improved Limb Atmospheric Spectrometer (ILAS) aboard the ADEOS (Advanced Earth Observing Satellite). The detection scheme for PSCs is based solely on ILAS visible channel transmittances in and around the A-band of molecular oxygen, without taking recourse to spectroscopic reference data or radiative transfer modeling. PSC presence and vertical extent are detected from linear fitting of transmittances outside the O<sub>2</sub> A-band as a function of altitude. PSC optical thickness is derived from the ratio of observed transmittances to those determined from fitting. The additional atmospheric light path arising from multiple scattering inside the cloud is obtained from the transmittances inside the O<sub>2</sub> A-band. Consideration of aerosol extinction coefficients retrieved independently from ILAS observations allows an estimate of the horizontal extent of the PSC. Comparisons with vertical profiles of nitric acid (HNO<sub>3</sub>) observed from ILAS show denitrification in altitude regions where PSCs are detected.

**P12. Analysis of the ILAS Limb Transmission Spectra at 753 - 784 nm:  
Comparisons on O<sub>2</sub>-A-band Line Parameters  
and Ozone Wulf Band Cross-sections**

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The Improved Limb Atmospheric Spectrometer (ILAS) aboard ADEOS (Advanced Earth Observing Satellite) measured profiles of chemical species in high latitudinal ozone layer about eight months from November 1996 to the end of June 1997 by a solar occultation method.

ILAS had a grating spectrometer whose spectral band covers 753 - 784 nanometers. This band, ILAS Visible channel, is designed to obtain vertical profiles of temperature and pressure (T/p) from O<sub>2</sub>-A-band spectra. We have faced several problems to retrieve T/p profiles from the ILAS data. Major items of them are: the ILAS instrument function, tangent height determination, O<sub>2</sub>-A-band line parameters, and ozone Wulf band cross-sections. The former two items have been almost resolved.

As for the O<sub>2</sub>-A-band line parameters, we have investigated and compared between the HITRAN'96 and the new parameters from Dr. L. Brown. Brown's data<sup>1</sup> seem to be better from the ILAS test retrieval results of T/p.

We do not have sufficient ozone Wulf band cross-section data. We have tested the data from MODTRAN3.5 and Dr. J.P. Burrows's data.<sup>2</sup> There seems to be several problems on temperature dependency and spectral features judged from the results of base-line fitting of the ILAS measurement data.

The present status of data analysis on the ILAS Visible channel is reported here.

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1. L.R. Brown and G. Plymate, *J. Mol. Spectrosc.* **199**, 166-179 (2000).

2. J.P. Burrows et al, *J. Quant. Spectrosc. Radiat. Transfer* **61**, 509-517 (1999).

### **P13. HITRAN Considerations for HIRDLS**

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The HIRDLS (High-Resolution Dynamics Limb Sounder) radiometer will make measurements of IR limb emission from the EOS (Earth Observing System) Aura platform due for launch in the summer of 2003. The instrument uses 21 channels covering the spectral range from 6.1 to 17.8 micrometers and science products will include temperature, O<sub>3</sub>, H<sub>2</sub>O, CH<sub>4</sub>, N<sub>2</sub>O, NO<sub>2</sub>, HNO<sub>3</sub>, N<sub>2</sub>O<sub>5</sub>, CFC11, CFC12, ClONO<sub>2</sub>, aerosols, the locations of polar stratospheric clouds and cloud tops, and geopotential height gradients. Retrieval accuracy will depend on knowledge of spectral line parameters, heavy molecule cross-sections, and aerosol refractive indices for the channel target and interfering species. In this presentation we will discuss particular concerns with respect to the current HITRAN database as it impacts retrieval accuracy and our ability to meet the HIRDLS science objectives. For example, an important region scientifically is the upper troposphere/lower stratosphere where temperatures can fall below 200 K. This is a potential problem since the quality of spectral data is generally poorer at lower temperatures. We make suggestions for future spectroscopic measurements and modeling that would be of benefit to HIRDLS with the aim of promoting interaction between the spectroscopic and remote-sounding communities.

## **P14. The ISSWG Line-by-Line Intercomparison**

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A short poster presentation is proposed where the Line-by-line model Intercomparison Exercise (LIE) in support of the IASI (Infrared Atmospheric Sounding Interferometer) mission is described. If possible, some initial results will be discussed as well. The objective of LIE was to document agreement and differences among line-by-line models. This will be achieved from an intercomparison of a number of different line-by-line models for a limited number of scenarios. Two cases involved a comparison with observations by HIS (High-resolution Interferometer Sounder) and ARIES (). In total, eleven research groups participated in the LIE.

**P15. Spectroscopic Requirements for MIPAS/ENVISAT non-LTE Analysis****Bernd Funke,<sup>a</sup> Francisco J. Martin-Torres,<sup>a</sup> Gabriele P. Stiller,<sup>a</sup>  
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High-resolution emission spectra to be measured by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on ENVISAT in the mid-IR will enable the retrieval of relevant atmospheric trace gases from the upper troposphere up to the lower thermosphere. However, many ro-vibrational states of the emitting species depart from local thermodynamic equilibrium (LTE) in a wide altitude range. The analysis of non-LTE affected spectra requires more spectral information than under LTE conditions for two reasons: First, hot band emissions, which are too weak to be detected under LTE, strongly contribute to measured spectra due to increased non-LTE populations of high energetic levels. Second, the retrieval of atmospheric species from emission spectra requires the calculation of non-LTE populations under consideration of all relevant radiative processes. On the other hand, the accurate non-LTE analysis of MIPAS data under support of an extended spectral database would offer unprecedented information for testing non-LTE models, for improving our knowledge of non-LTE mechanisms and heating/cooling processes in the atmosphere. Available spectral databases such as HITRAN contain line parameters for most of the important atmospheric bands. However, for some molecules such as O<sub>3</sub>, NO, CH<sub>4</sub>, and NO<sub>2</sub> these compilations do not cover all transitions which contribute to measured spectra under non-LTE or which are needed for the proper modelling of non-LTE populations. In the case of O<sub>3</sub>, information about the  $\nu_1$ ,  $\nu_2$ ,  $\nu_3$ , and  $\nu_1+\nu_3$  hot bands, emitting in the 4.8  $\mu\text{m}$  and 10  $\mu\text{m}$ , originating from very high-energetic vibrational levels is needed. In order to account for superthermal non-LTE emissions of thermospheric NO, information on ro-vibrational  ${}^2\Pi_{\Omega}(v) \rightarrow {}^2\Pi_{\Omega}(v-1)$  lines with  $J > 35.5$  is required. Pure rotational transitions of OH in the 8 - 30  $\mu\text{m}$  region are missing in the HITRAN96 edition. For CH<sub>4</sub> there is poor spectroscopic information about the levels emitting in the 1.7- $\mu\text{m}$ , 2.3- $\mu\text{m}$ , and 3.3- $\mu\text{m}$  regions, which cannot be measured directly by MIPAS but which might have a strong influence in the 7.6  $\mu\text{m}$  and 6.5  $\mu\text{m}$  CH<sub>4</sub> emissions via collisional and radiative cascade. Also, spectroscopic information about the NO<sub>2</sub>  $\nu_3$  hot bands is required. The aim of this poster is to assess the spectroscopic requirements necessary for the accurate non-LTE analysis of MIPAS/ENVISAT data.

## **P16. Requirement for Refractive Indices for MIPAS/ENVISAT PSC Analysis**

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MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) will be operated on board of ESA's polar orbiting satellite ENVISAT foreseen to be launched in mid-2001. The instrument will perform limb measurements with 3-km vertical spacing from about 6 km to 68 km altitude. Its spectral resolution of  $0.035 \text{ cm}^{-1}$  is unprecedented for broadband mid-infrared emission measurements from space. Due to MIPAS' capability to measure during night and its good coverage of the Arctic and Antarctic regions, a main target of the experiment is to investigate the composition of the wintertime polar stratosphere. Up to a tangent altitude of around 30 km, polar stratospheric clouds (PSCs) will affect the measured spectra in the cold stratospheric vortex. While this might render the retrieval of atmospheric trace gases more difficult, it offers the opportunity to extract PSC microphysical information from the spectra. Within the scope of developing a scientific processor for the retrieval of atmospheric parameters from MIPAS-ENVISAT measurements we have investigated the influence of PSCs on limb spectra.

Optical constants of aerosols are one input quantity of the Mie model. Since the composition of PSCs is still under discussion, we have collected the available laboratory measurements of optical constants for the various chemical compositions. A comparison of the different data sets shows that even for the same substances large differences occur. For typical size distributions limb spectra in the five MIPAS bands have been simulated using the various laboratory optical constants for ice, NAD, NAT,  $\text{H}_2\text{O}/\text{HNO}_3$ ,  $\text{H}_2\text{O}/\text{H}_2\text{SO}_4$  and  $\text{H}_2\text{O}/\text{HNO}_3/\text{H}_2\text{SO}_4$  solutions of different composition. The differences of these simulations will be shown highlighting the need for more accurate refraction indices of some of the examined aerosol types.

**P17. The Need for Water and Methane Spectroscopic Data  
for the Interpretation of SCIAMACHY Near-infrared Measurements**

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The atmospheric spectrometer SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartography), to be launched in 2001 on board ESA's ENVISAT satellite, will allow the measurement of atmospheric absorption spectra from the ultraviolet to the near infrared (240–2400 nm) with resolutions down to 0.2nm FWHM. Spectra can be obtained in nadir, limb, and occultation observation modes. The instrument features novel InGaAs detectors for the near infrared wavelength range. In the spectral region covered by SCIAMACHY's longest wavelength channel (2265 - 2380 nm) absorption lines of water, methane, carbon monoxide, and nitrous oxide are present. Therefore, SCIAMACHY measurements will provide global information on the distribution of these gases in the atmosphere. Since the lines of carbon monoxide and nitrous oxide are an order of magnitude fainter than the stronger water and methane lines, the accuracy of the determination of concentrations of the former gases depends on the quality of the spectroscopic knowledge of methane and water in the regions overlapping carbon monoxide and nitrous oxide lines.

## **P18. Lidar Equation Modeling Using LIDAR-PC and the HITRAN Database**

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A computer program , LIDAR-PC, has been developed to simulate the LIDAR Equation using the HITRAN database for atmospheric molecular attenuation and the LOWTRAN/BACKSCAT program for aerosol attenuation and backscatter. The program computes the return for hard and aerosol targets as a function of altitude, and uses the HITRAN-PC computer program to generate a wavelength vs altitude profile of the atmosphere. Details and examples of the interplay of the HITRAN database and lidar calculations for Differential Lidar calculations will be shown. The programs are being distributed by the ONTAR Corp.

## Rotational Spectroscopy in Support of Upper Atmospheric Research at JPL

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Rotational spectroscopy at JPL supports the NASA's Upper Atmospheric Research Program by providing a database of rotational transitions and by performing laboratory measurements to improve the database as required by the observational programs. Of prime concern are the spectroscopic needs of the EOS-MLS (Earth Observing System – Microwave Limb Sounder) experiment. Because air-broadened linewidth measurements of rotational transitions are sparse, the JPL compilation of rotational spectra does not include any linewidth information. Several of the transitions that will be observed by EOS-MLS will require improved accuracy of their linewidth parameters. The MLS requirements will be presented and the laboratory program to satisfy the requirements will be described. Current measurements of the HCl  $J = 1 - 0$  transition near 625.9 GHz will be used to illustrate the work in progress. These measurements will be compared to those of the corresponding transition in the vibrational spectrum and to measurements made in other laboratories.

Because of the role of the halogen oxides in upper atmospheric processes resulting in ozone depletion, our studies are also directed toward better determination of their molecular properties as well as their spectra. Recently we have extended the range of observations of ClO, BrO, and IO. In the process of these investigations, we discovered that we were able to generate IO and BrO in highly excited vibrational states,  $\nu = 13$  in  $X_1^2\Pi_{3/2}$  and  $\nu = 9$  in  $X_2^2\Pi_{1/2}$  for IO and  $\nu = 8$  in  $X_1^2\Pi_{3/2}$  and  $\nu = 7$  in  $X_2^2\Pi_{1/2}$  for BrO. In addition, we used  $^{18}\text{O}$  enrichment to observe the isotopically-substituted molecules. For ClO the excitation mechanisms which were effective in the heavier oxides do not seem to occur. However, ClO is generated in high yield and we were able to observe  $\nu = 2$  spectra at thermal populations and  $^{18}\text{O}$  spectra in natural abundance. Isotopically independent parameters will be presented for ClO, BrO and IO and interpreted in terms of their interatomic potentials and electron distributions.

OIO was discovered as a byproduct of the IO reactions. These were the first high-resolution observations of OIO. As is the case for OClO and OBrO, OIO has a  $^2B_1$  ground electronic state. Both the ground vibrational state and first excited bending state spectra of the  $X^2B_1$  state have been analyzed. Thus, precise molecular parameters are now available for the series of compounds, OClO, OBrO and OIO. Their structures and electron distributions will be compared.

Related compounds for which spectra have been analyzed include ClOClO<sub>2</sub>, ClClO<sub>2</sub>, HOClO<sub>3</sub> (perchloric acid), and FClO. The status of the halogen oxide spectra included in the JPL database will be discussed.

## A New Spectroscopic Database for the Ozone Fundamentals

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Mid-infrared measurements of ozone in the range 600 to 1300  $\text{cm}^{-1}$  have been performed with the high-resolution Bruker IFS 120 HR spectrometer. 16 measurements were recorded at 0.2 to 9 mbar ozone pressure, 0 to 40 mbar air pressure, 200 to 296 K temperature and 0.0011 to 0.0022  $\text{cm}^{-1}$  spectral resolution, depending on air pressure, applying a cell with a 25-cm absorption path. Line positions and line strengths were retrieved from pure ozone measurements while pressure broadening parameters and temperature exponents were obtained from all measurements. Quantum mechanical analysis was performed for line positions and linestrengths. Polynomial expansions in the  $m$  quantum number for different sets of  $K_a$  subbands were applied for data reduction of pressure broadening parameters and temperature exponents. A new database in HITRAN format was produced and quality assured by means of comparison of modelled and measured laboratory and solar occultation atmospheric spectra. Comparison with HITRAN96 revealed significant differences for the pressure broadening data, the band strengths differed by about 3%.

## High-Resolution Analysis of H<sub>2</sub>CO in the 3.6- and 4.3-micrometer Regions

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Using new Fourier transform spectra recorded at high resolution at LPMA Paris, it has been possible to perform an extensive study of the formaldehyde absorption spectra in the 2600-3000 cm<sup>-1</sup> and in the 2200-2500 cm<sup>-1</sup> spectral ranges. This analysis was started using the results obtained previously in the same spectral regions<sup>1,2</sup> and using the ground state parameters of Muller et al.<sup>3</sup> In this way, more than 10000 lines were identified which belong to 10 bands of formaldehyde. From this analysis it appears that these bands cannot be considered as independent.

In the high-frequency range, the analysis of the strongest bands, namely  $\nu_1$  and  $\nu_5$  (symmetric and antisymmetric stretching modes), was complicated by the existence of Fermi-type resonances and by A-type, B-type and C-type Coriolis interactions with various overtone or combination states, namely  $\nu_2+\nu_6$ ,  $2\nu_3$ ,  $\nu_2+\nu_4$ ,  $\nu_3+\nu_6$ , and  $\nu_3+\nu_4$ .

The analysis was further complicated by additional perturbations due to the weak  $2\nu_4$  and  $2\nu_6$  bands and to the very weak  $\nu_4+\nu_6$  band which appear in the low frequency range. The final calculation which involves about 2900 levels belonging to 10 different vibrational states leads to rather reasonable results, given the difficulty of the problem.

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## The Venus 1-mm CO<sub>2</sub> Bands and the O<sub>2</sub> (0-1) X<sup>3</sup>Σ<sub>g</sub><sup>-</sup> - a<sup>1</sup>Δ<sub>g</sub> and (1-0) X<sup>3</sup>Σ<sub>g</sub><sup>-</sup> - b<sup>1</sup>Σ<sub>g</sub><sup>+</sup> Bands in the Earth's Atmosphere

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The Venus CO<sub>2</sub> band triad in the 9300-9700 cm<sup>-1</sup> region has been observed in new near infrared 0.05 cm<sup>-1</sup> resolution ground-based solar absorption spectra, obtained in the 9000-12000 cm<sup>-1</sup> region, at large solar zenith angles. Considering the available line positions and pressure line shifts for CO<sub>2</sub>, H<sub>2</sub>O and O<sub>2</sub> in this region, it is concluded that the new observations show significant inconsistencies among the line positions of these species as listed in the atmospheric spectroscopy databases. The new spectra also allow a better definition of the O<sub>2</sub> (0-1) X<sup>3</sup>Σ<sub>g</sub><sup>-</sup> - a<sup>1</sup>Δ<sub>g</sub> band, with the discrete (0-1) transitions observable in the 9300-9450 cm<sup>-1</sup> region, superimposed on a collision-induced continuum covering the 9200-9700 cm<sup>-1</sup> region. This continuum, as well as the (0-0) continuum in the 7900 cm<sup>-1</sup> region, have been previously studied only from atmospheric spectra with much lower spectral resolution. The discrete O<sub>2</sub> (1-0) transitions of the X<sup>3</sup>Σ<sub>g</sub><sup>-</sup> - b<sup>1</sup>Σ<sub>g</sub><sup>+</sup> band are observed in the 11500-11600 cm<sup>-1</sup> region, but no evidence is found for an underlying continuum.

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## Characterization of the $\nu_3$ Band of Methane

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The  $\nu_3$  band of methane is an important tool for studies of the Earth's atmosphere by instruments such as the HALogen Occultation Experiment (HALOE). It has long been realized that the HITRAN parameters do not adequately represent the atmospheric spectrum, but improvement has proved very difficult. Line mixing is the cause of this problem and the lines that are mixing are frequently close enough to each other that the Rosenkrantz approximation is not adequate. The full relaxation matrix formulation is required. Since some experiments, HALOE in particular, involve a cell filled with methane, characterization of the spectrum for self broadening is also required. Traditional single spectrum analysis is able to derive line mixing only in the Rosenkrantz approximation. We have undertaken a project to reanalyze the  $\nu_3$  band system of methane near  $3000\text{ cm}^{-1}$  using over 60 spectra with the multispectrum fitting technique of Benner et al.<sup>1</sup> Self- and air-broadening, shifting and mixing are included and the temperature dependence for air induced parameters have also been measured for the stronger transitions. The HITRAN format lacks some of the required parameters to characterize the spectrum, namely self induced pressure shift coefficients, temperature dependence of the air induced pressure shift, self and air induced off-diagonal relaxation matrix elements, and the temperature dependence of the air induced off-diagonal relaxation matrix elements. The off-diagonal relaxation matrix elements and their temperature dependence are a particular problem for the HITRAN style of spectral line list since these parameters are not tied to a single transition, and a single transition may have more than one set of these coefficients.

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## Infrared Spectroscopy of Ammonia $^{14}\text{NH}_3$

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The interest in high resolution infrared studies of ammonia,  $\text{NH}_3$ , has recently increased, motivated by the need for more spectroscopic parameters for this molecule, such as line positions, intensities and widths required in the analysis of the high-quality planetary spectra recently obtained in the Jupiter and Saturn atmospheres by the SWS (Short Wavelength Spectrometer) of the ISO satellite and by the NIMS (Near Infrared Mapping Spectrometer) of the Galileo Spacecraft. In this talk, we will try to review some of the results obtained over the last few years on the high-resolution infrared spectroscopy of ammonia.

Ammonia is the good example of a non-rigid molecule, showing a large amplitude motion, well-known as the inversion. As a consequence of the relatively low double minimum potential function that separates equivalent pyramidal configurations, the molecule oscillates between those two configurations. The quantum mechanical tunneling through the potential barrier results in a splitting of the energy levels that, in its turn, is responsible for a splitting of the lines visible in the spectra.

A rather large spectral range of the infrared spectra of ammonia, from about 900 to 3600  $\text{cm}^{-1}$ , corresponding to different polyads of vibrational-inversional-rotational states, has been studied extensively. Between 5 and 7  $\mu\text{m}$ , the  $2\nu_2$  (overtone of the inversion mode  $\nu_2$ )/ $\nu_4$  (fundamental bending mode) system is involved. At 4  $\mu\text{m}$ , the dyad  $3\nu_2/\nu_2+\nu_4$  is considered and in the 3- $\mu\text{m}$  region, a more complex interacting system involving the fundamental stretching band  $\nu_1$ , the  $\nu_3$  bending mode and the overtone  $2\nu_4$  has been studied. Various hot bands are also investigated to complete the 3  $\mu\text{m}$ , 4  $\mu\text{m}$  and 5-7  $\mu\text{m}$  studies. Above 3600  $\text{cm}^{-1}$ , the polyads become more complex and the understanding of the infrared data is far from being complete.

The first part of the talk will concentrate on recent progress made in the 1200-3600- $\text{cm}^{-1}$  range. The experimental data, both in frequency and in intensity, recorded mainly using the Fourier Transform Spectrometers located at the Kitt Peak Observatory and at the Jet Propulsion Laboratory (JPL, Pasadena, USA) will be presented. Then I will briefly describe the method used to analyze the infrared spectra of ammonia. The theoretical approach, based on the literature, takes into account not only the inversion phenomena which cannot be treated like any other small amplitude motion by the usual methods, but also the different interactions (Coriolis type or Fermi type) that occur in a given dyad or triad. The existing data set has been thus recently updated and will be submitted to the HITRAN database.

Our results will be illustrated in the different spectral ranges and finally some of the limitations and drawbacks of our approach will be discussed.

## Benchmark Laboratory Methanol Data at the University of New Brunswick, Canada

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The spectroscopy of methanol has acquired great importance in a wide number of areas and applications in recent years. At the University of New Brunswick, we are engaged in a broad range of experimental and theoretical studies of the spectroscopy of methanol and its isotopomers. Our investigation can be grouped in the following principal categories: 1. Methanol and most of its isotopomers have been systematically studied in the MW and FIR regions for the ground state. Recently, efforts have been directed successfully towards global modeling of the first two torsional levels using a one-dimensional large-amplitude Hamiltonian<sup>1</sup> in order to obtain reliable molecular parameters, ground-state energies and transition strengths, and to consolidate our extensive ground-state information to be most useful to the astronomical community. 2. The CO-stretch fundamental overlaps well with the CO<sub>2</sub> laser bands so has important application for IR pumping of FIR lasers. To extend the range of IR tuning coincidences, almost every existing methanol isotopomer has been examined exhaustively for CO<sub>2</sub>-pumped FIR laser emission. So far, the CO-stretch spectra also have been studied for the majority of the isotopomers, allowing us to contribute extensively to identification of the laser transitions. 3. Above the strong CO-stretch fundamental in methanol lies a broad and ambiguous region of weak bands including the methyl rock and deformation and the OH bend. We are now making steady progress in this rich but messy region of long-standing mystery in terms of subband analysis. However, the question of the detailed vibrational and even torsional assignment of the upper-state levels sometimes remains undetermined. 4. Most recently, the 3- $\mu\text{m}$  methanol spectral bands have been revisited with both molecular beam and FT techniques, and a more complete energy picture with substantial *K* coverage is now emerging. A driving force behind this is the dramatic observations of these bands in recent comets and the increased needs from the cometary community. It is fair to say that the ground state of methanol is largely under control, providing firm ground for IR band analysis. In contrast, among the assigned fundamental bands, only three have any degree of compromise with the existing 1-D torsional Hamiltonian. Average obs.-calc. residuals of 0.02, 0.04 and 0.08  $\text{cm}^{-1}$  are obtained for the 10- $\mu\text{m}$  CO-stretch  $\nu_8$ , the 3.3- $\mu\text{m}$  symmetric CH-stretch  $\nu_3$ , and the 2.7- $\mu\text{m}$  OH-stretch  $\nu_1$  bands, respectively, when localized substates are excluded from the fits. On the other hand, four bands present a mirror image of the expected pattern. The two asymmetric CH-stretch modes  $\nu_2$ ,  $\nu_9$ , the asymmetric CH-bend  $\nu_4$  and the out-of-plane CH<sub>3</sub> rock  $\nu_{11}$  all display inverted torsional structure, representing a complete breakdown of the usual 1-D model. We are not satisfied with this situation. Thus, *ab initio* tools are being adapted to

explore the torsional dependence of atomic displacements and vibrational force constants. This should give the information needed to model the methanol fundamentals with a newly designed formalism.<sup>2</sup>

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**P19. Some New Laboratory Measurements  
and their Effect upon the Spectroscopic Database**

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Measurements on various molecular bands listed in the HITRAN and GEISA databases have been performed in our laboratory. The results seem to suggest some improvements that can be made in the current compilations. The molecules in question are H<sub>2</sub>O, CO, CO<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, NH<sub>3</sub> and N<sub>2</sub>O.

**P20. Methane Line Parameters in the MOPITT Channels  
near 2.3 mm (2300 nm)**

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The line intensities and air- and self-broadened Lorentz widths and pressure-induced shifts have been measured for methane from 4262 to 4305  $\text{cm}^{-1}$  and 4352-4500  $\text{cm}^{-1}$ . Seven spectra of  $^{12}\text{CH}_4$  and four spectra of air + methane were recorded at 0.012  $\text{cm}^{-1}$  resolution using the McMath Fourier-transform spectrometer located at Kitt Peak. Nearly 1000 transitions of the three strongest bands  $\nu_1+\nu_4$ ,  $\nu_3+\nu_4$  and  $\nu_2+\nu_3$  were retrieved simultaneously from the eleven scans using the multi-spectrum fitting program. These measurements support the atmospheric remote sensing being done by the MOPITT (Measurements of Pollution in the Troposphere) experiment currently in orbit on the TERRA satellite.

**P21. Air-, N<sub>2</sub>- and Self-Broadening and Shift Coefficients and Line Mixing in the ν<sub>3</sub>, ν<sub>5</sub> and ν<sub>6</sub> Bands of <sup>12</sup>CH<sub>3</sub>D**

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We have measured Lorentz broadening coefficients and pressure-induced shift coefficients for more than 1500 transitions in the ν<sub>3</sub>, ν<sub>5</sub>, and ν<sub>6</sub> fundamental bands of <sup>12</sup>CH<sub>3</sub>D in the spectral region from about 1000 to 1600 cm<sup>-1</sup>. A total of 26 room-temperature absorption spectra of 98% enriched CH<sub>3</sub>D and CH<sub>3</sub>D mixtures with air and nitrogen were recorded at 0.006 cm<sup>-1</sup> resolution with the McMath-Pierce Fourier transform spectrometer (FTS) of the National Solar Observatory on Kitt Peak and at 0.002 cm<sup>-1</sup> resolution by a Bruker IFS 120 HR at PNNL. Sets of 11 to 17 of these spectra were simultaneously analyzed using a multispectrum nonlinear least squares fitting technique.<sup>1</sup>

In each band we determined air-,<sup>2-4</sup> N<sub>2</sub>- and self-broadening and shift coefficients for hundreds of transitions with rotational quantum numbers up to  $J^2 = 15$  and  $K^2 = 15$ . Some forbidden transitions with  $|DK| > 1$  were also analyzed. Weak line mixing effects were observed in some high- $J$  transitions with  $K^2 = 3$  in all three bands, and we have determined off-diagonal relaxation matrix element coefficients for their  $AIA2$  split components.

Empirical expressions have been determined to model the observed variations of the measured parameters with vibrational and rotational quantum numbers. We will compare our results with the values on the 1996 HITRAN compilation<sup>5</sup> and with other available measurements.

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## P22. Recent Progress Achieved in the 6.2-mm Region for Nitrogen Dioxide

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This paper will present recent progress achieved for NO<sub>2</sub> line position and intensity parameters in the 6.2-micrometer region. The 6.2-micrometer region corresponds to the strongest infrared band,  $\nu_3$ , of this molecule and is therefore widely used for atmospheric measurements of nitrogen dioxide in the stratosphere or upper troposphere. As compared to the previous update performed in 1998 for nitrogen dioxide in the HITRAN database,<sup>1,2</sup> we present new progress concerning, on the one hand, the  $\nu_3$  band for the <sup>15</sup>NO<sub>2</sub> isotopic species and, on the other hand, the 3 $\nu_3$ -2 $\nu_3$  hot band for the main isotopic species.

### 1- The $n_3$ band for the <sup>15</sup>NO<sub>2</sub> isotopic species:

New high-resolution Fourier transform absorption spectra of an <sup>15</sup>N<sup>16</sup>O<sub>2</sub> isotopic sample of nitrogen dioxide were recorded at the University of Bremen in the 6.3-micrometer region. Starting from the results of a previous study,<sup>3</sup> a new and extended analysis of the  $\nu_3$  band located at 1582.1039 cm<sup>-1</sup> has been performed.

### 2- The 3 $n_3$ -2 $n_3$ of hot bands for the <sup>14</sup>NO<sub>2</sub> isotopic species:

The goal of this analysis was to generate line parameters for the 3 $\nu_3$ -2 $\nu_3$  hot band of nitrogen dioxide. This work was motivated by the results<sup>4</sup> from the Limb Infrared Monitor of the Stratosphere (LIMS) instrument suggesting that Non-Local Thermodynamical Equilibrium (NLTE) may result in emission due to hot bands of NO<sub>2</sub>. It is surmised that in the analysis of higher spectral resolution data of future remote sensing instruments, such as MIPAS, the NLTE emission of such hot bands may be of significance in the interpretation of the resulting data. Using high-resolution Fourier transform spectra of nitrogen dioxide measured in the 2-micrometer region at the University of Denver, it has been possible to perform the analysis of the 3 $\nu_3$  band. From these results, the 3 $\nu_3$ -2 $\nu_3$  hot band was generated using for the intensity calculation a realistic transition moment operator.

In both studies, the spin-rotation line positions and intensities were satisfactorily calculated using a theoretical model that takes into account both the Coriolis interactions and the spin rotation resonances.

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## P23. Positions and Intensities of Ammonia Hot Bands in the 4- to 8-mm Region

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To complete our infrared analyses of  $^{14}\text{NH}_3$  between 5 and 8  $\mu\text{m}$ ,<sup>1</sup> a region dominated by the absorption of the  $2\nu_2$  overtone and  $\nu_4$  fundamental bands, we have also analyzed the  $3\nu_2 - \nu_2$  and  $\nu_2 + \nu_4 - \nu_2$  hot-band line positions and intensities measured at 0.005  $\text{cm}^{-1}$  resolution with the Fourier transform spectrometer located at the Kitt Peak National Observatory. Using the  $\nu_2 = 3$  and  $\nu_2 = \nu_4 = 1$  upper states energy obtained previously,<sup>2</sup> several hundred line positions with  $J$  up to 10 have been assigned to the  $3\nu_2(\text{s}) - \nu_2(\text{a})$ ,  $3\nu_2(\text{a}) - \nu_2(\text{s})$ ,  $\nu_2 + \nu_4(\text{s}) - \nu_2(\text{s})$  and  $\nu_2 + \nu_4(\text{a}) - \nu_2(\text{s})$  located around 1416, 1963, 1608 and 1618  $\text{cm}^{-1}$  respectively. Some 269 intensity measurements have been analyzed to about 7%. In the 4  $\mu\text{m}$  region, which is dominated by the absorption of the  $3\nu_2$  overtone and the  $\nu_2 + \nu_4$  combination band, we have found a number of lines belonging to the hot bands  $\nu_1 - \nu_2$ ,  $\nu_3 - \nu_2$  and  $2\nu_4 - \nu_2$  using the upper state energy parameters determined in our previous study in the 3  $\mu\text{m}$  region.<sup>3</sup> We have confirmed assignments involving the  $4\nu_2(\text{s})$  overtone centered around 3462  $\text{cm}^{-1}$  by identifying  $4\nu_2 - \nu_2$  transitions. This work provides a first analysis of ammonia hot bands near the 5  $\mu\text{m}$  window being used to monitor atmospheres of planets and cool stars.<sup>4</sup>

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**P24. HBr and HI Line Parameters Update  
for Atmospheric Spectroscopy Databases**

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Recent work on new line parameters for the  $X^1\Sigma^+$  (0-0),(0-1)  $H^{79}\text{Br}$ ,  $H^{81}\text{Br}$  bands and the  $X^1\Sigma^+$  (0-0),(0-1) HI bands, which include hyperfine structure, has been extended for an update of spectroscopic databases in use for atmospheric spectroscopy.

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**P25. Updated Electric Dipole-Moment Function  
for the Ground Electronic State of Carbon Monoxide**

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The electric dipole moment function of the ground electronic state of carbon monoxide has been redetermined so as to reflect the most up-to-date laboratory measurements of individual rovibrational line intensities of various vibrational transitions. This function will then be used to update the rovibrational line intensities given by HITRAN as well as HITEMP.

**P26. A Multispectrum Fitting Procedure  
to Improve the Accuracy of Line Parameters.  
Application to the Second Overtone of CO: Preliminary Results**

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A few teams<sup>1,2</sup> have developed least-squares fitting procedures able to treat simultaneously several laboratory spectra in order to deduce line parameters. Many advantages were found in this technique, such as the possibility to fit spectra obtained at different resolutions or recorded with different spectrometers, or the ability to obtain parameters that cannot be determined from a single spectrum, and also an improvement of the statistical uncertainties compared with the usual spectrum-by-spectrum procedure.

With the aid of a Gauss-Newton-like algorithm which does not use derivatives to perform the non-linear least-squares adjustment, we are extending a previous automatic method<sup>3</sup> in order to treat simultaneously several FT spectra. The adjustable or fixed parameters are, first of all, those of the involved lines (positions at zero pressure, pressure-shifting and broadening coefficients, collisional-narrowing coefficients if needed, and intensities): they are constrained at the same value in all the spectra; and, second, some parameters depending upon the spectrum (effective iris radius, phase error if needed, and level, slope, and curvature of the continuous background). A work is in progress to validate this procedure with the aid of FT spectra of the 3–0 band of <sup>12</sup>C<sup>16</sup>O, recorded under a 0.006 cm<sup>-1</sup> resolution and pressures between 4 and 760 Torr, and which had already been used to measure absolute wavenumbers and self-pressure shifts,<sup>4</sup> as well as line intensities and self-broadening coefficients.<sup>5</sup>

At this stage of the work, this procedure appears versatile and is found powerful and significantly time-saving in the data reduction. It is able to treat a slight collisional narrowing, observed for the first time for CO in FT spectra. Some problems occur when the wavenumber scales of the spectra cannot be accurately calibrated, but it is easy to get around this drawback by letting free the line positions in each spectrum; then, even in this case, the multispectrum technique keeps its interest.

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## P27. Revisited Line Intensities of Acetylene $^{12}\text{C}_2\text{H}_2$ in the 13.6-mm Spectral Region

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Acetylene is present both in the terrestrial troposphere, and in the urban atmosphere as a pollutant. Lines absorbing in the 13.6  $\mu\text{m}$  region were observed in Denver University balloon flight spectra in 1981, from which Goldman et al<sup>1</sup> deduced that  $\text{C}_2\text{H}_2$  is present in a very small amount in the upper troposphere (about 25 pptv at 9 km altitude in 1981 and rapidly increasing since). Acetylene is also present in trace amounts in the upper atmosphere of the giant planets, where it comes from the methane photodissociation, and is observable in emission spectra through the strong  $Q$ -branch of the  $\nu_5$  band.

As it is important for applications, the  $\nu_5$  band region has been the subject of numerous studies. Line positions are known with accuracy and can be found in the HITRAN database, where line intensities, from the work of Weber et al,<sup>2</sup> are also given. Measurements of line intensities, as well as nitrogen and hydrogen broadening coefficients, especially at planetary atmospheric temperatures, were recently performed by Sun and Varanasi.<sup>3</sup>

In the present work,<sup>4</sup>  $\text{C}_2\text{H}_2$  spectra were obtained with the LPMA interferometer, at an apodized resolution limit of  $0.0014\text{ cm}^{-1}$ . Absolute intensities were measured for more than 430 lines belonging to the  $\nu_5$  band and five hot bands, with an accuracy of  $\pm 5\%$ , allowing the determination of the vibrational transition dipole moments squared and Herman-Wallis coefficients. On the whole, our intensities agree well with the recent values obtained by Sun and Varanasi<sup>3</sup> for the  $\nu_5$  band (4 % average difference), whereas they are found greater than those available in HITRAN 1996 by about 14 %.

These results will be presented and compared with other existing experimental values. Special attention will be paid to the procedure used to retrieve accurate absolute intensities from the spectra. Particularly, the importance of the throughput in the apparatus function, and its non negligible dependency vs wavenumber, will be carefully discussed.

Based upon our line intensities, a synthetic spectrum has been generated in the HITRAN format and will be included in the next issue.

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**P28. Intensity and Linewidth Measurements in the 13.7-mm Bands of C<sub>2</sub>H<sub>2</sub> at Planetary Temperatures**

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Measurements of spectral line parameters are reported on the  $\nu_5$ -fundamental band region. Employing a Bruker 120-HR Fourier transform spectrometer we have measured line strengths, H<sub>2</sub> and N<sub>2</sub> broadening line widths, and pressure-induced line shifts at temperatures between 150K and 296K. The dependence of the line widths upon temperature will be discussed along with the distribution of the line intensities amongst the various hot bands located in this spectral region.

**P29. Absolute Line-Intensity Measurements in the  $\nu_2$  Band of HOCl**

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We have measured absolute line intensities in the  $\nu_2$  fundamental band at  $1238\text{ cm}^{-1}$  of both isotopomers of hypochlorous acid. To obtain the partial pressure of the species in the sample mixture, unavailable through direct measurement since HOCl exists only in equilibrium with  $\text{H}_2\text{O}$  and  $\text{Cl}_2\text{O}$ , we relied on known line intensities in the pure rotational far infrared spectrum determined from Stark effect measurements. We have thus recorded *simultaneously* the FIR pure rotation spectrum of HOCl using a Bruker IFS120HR interferometer and the spectrum of a few vibration-rotation lines in the infrared IR  $\nu_2$  band using a tunable diode laser spectrometer. The absolute intensities of these IR lines thus determined allowed us to calibrate the intensities of vibration-rotation lines in the whole band, measured using Fourier transform spectroscopy. The treatment of the data took into account the blackbody emission contribution in the FIR and the evolution of the HOCl amount during the recording of the spectra. The square of the transition dipole moment and a linear Herman-Wallis factor were determined for both isotopomers. The line intensities were also least-squares fitted using a full model that calculates explicitly the transition moment matrix elements. This allowed us to account for a weak resonance between the 010 and 002 levels, which leads to the observation of a few  $2\nu_3$  resonating lines. The experimental work, results and comparison with previous measurements will be presented.

## **P30. A New Spectroscopic Database for Chlorine Nitrate**

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Mid-infrared measurements of chlorine nitrate have been performed with the high-resolution Bruker IFS 120 HR spectrometer. 29 measurements were recorded at 0.3 to 1 mbar chlorine nitrate pressure, 0 to 150 mbar air pressure, 190 to 296 K temperature and 0.0009 to 0.008  $\text{cm}^{-1}$  spectral resolutions, depending on air pressure, applying a cell with 25 cm absorption path. Particle density was deduced from pressure measurements of the purified sample which was synthesized from  $\text{N}_2\text{O}_5 + \text{Cl}_2\text{O}$ . Special attention was paid to quality assurance aspects. Absorption cross-sections were calculated from the spectra and a procedure was elaborated for temperature and air pressure interpolation. Significant differences to existing data were observed.

**P31. Absolute Absorption Cross-Section Measurements of the Schumann-Runge Continuum of O<sub>2</sub> at 78K and 295K**

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Laboratory measurements of the absorption cross-section of the Schumann-Runge continuum of O<sub>2</sub> at the temperatures 78K and 295K have been made in the wavelength region 130–175 nm. The absolute absorption cross sections at the same temperatures have been measured at several discrete wavelength region. The absolute cross sections of O<sub>2</sub> have been used to put relative cross sections on a firm absolute basis throughout the region 130–175 nm. These recalibrated cross-sections are available as numerical compilations.

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**P32. The Application of a VUV Fourier-transform Spectrometer and  
Synchrotron Radiation Source to  
Measurements of the  $\beta(6,0)$  and  $\gamma(3,0)$  Bands of NO**

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The  $\beta(6,0)$  ( $B\ 2\Pi_r - X\ 2\Pi_r$ ) and  $\gamma(3,0)$  ( $A\ 2\Sigma^+ - X\ 2\Pi_r$ ) bands of NO have been recorded using a VUV Fourier-transform spectrometer with synchrotron radiation as a light source. The analysis of the  $\beta(6,0)$  and  $\gamma(3,0)$  bands of NO provides accurate rotational line positions and term values. Molecular constants of the  $v = 9$  level of the  $B\ 2\Pi_r$  and  $v = 3$  level of the  $A\ 2\Sigma^+$  have been determined. Accurate rotational line strengths have also been obtained. The band oscillator strength of the  $\beta(6,0)$  and  $\gamma(3,0)$  bands are determined to be  $0.50 \times 10^{-4}$  and  $2.48 \times 10^{-4}$ , respectively.

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**P33. Predicted Predissociation Linewidths in the Schumann-Runge Bands of O<sub>2</sub> Compared with Recent High-Resolution Measurements****G.S-M. Tong,<sup>a</sup> Allan S-C. Cheung,<sup>a</sup> and Michael J. Jamieson<sup>b</sup>**

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We derive and use new parameters to quantify the semi-empirical expressions of Julienne and Krauss<sup>1</sup> for the  $^5\Pi_u$ ,  $^3\Sigma_u^+$ ,  $^3\Pi_u$  and  $^1\Pi_u$  potentials that predissociate the rovibrational levels of the  $B^3\Sigma_u^-$  state of O<sub>2</sub>. Using the new parameters in the model of Julienne and Krauss we evaluate fine-structure predissociation linewidths for the Schumann-Runge bands that terminate on the  $v = 13, 14$  rovibrational levels of the  $B^3\Sigma_u^-$  state. We compare these linewidths and those calculated with several existing sets of parameters with the measurements of Dooley et al<sup>2</sup> to demonstrate that the new values lead to improved agreement between theory and experiment. We also show the deperturbing effect of the level shifts, calculated with the new parameters, on the energies of the rotationless  $v = 0-17$  vibrational levels of the  $B^3\Sigma_u^-$  state.

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**P34. The Electronic Structure of NO<sub>2</sub><sup>+</sup>. An Ab-initio MRD-CI Study****Gabriel J. Vázquez<sup>a</sup> and Carolina Godoy<sup>b</sup>***<sup>a</sup>Centro de Ciencias Físicas, UNAM  
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We report ab-initio MRD-CI electronic structure calculations of the NO<sub>2</sub><sup>+</sup> cation. A basis set of DZ + POL quality augmented with *s*- and *p*-type Rydberg functions was employed together with an extensive treatment of electron correlation. Ten singlet and eight triplet states are calculated. The vertical ionization energies of NO<sub>2</sub> as well as bending and ON-O stretching potential energy curves of NO<sub>2</sub><sup>+</sup> are reported. Approximate vertical excitation energies of NO<sub>2</sub><sup>+</sup> are also reported. Several of the calculated states are reported for the first time. The vertical ionization spectrum of NO<sub>2</sub> is found in very good agreement with the experimental spectrum of Edquist et al.<sup>1</sup> Singlet-triplet splittings are reported and compared with the measured values.

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## Is the Water Molecule Spectroscopically Well Understood Now?

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The calculation of the ro-vibrational energy of isolated water molecules in the gas phase has been, for the past few years, the subject of a large number of investigations. These are mainly motivated by the spectroscopic importance of this molecule for a large number of areas such as, for instance, remote sensing of the earth's atmosphere. The calculation of the rovibrational energy of water is theoretically challenging since, due to the lightness of the hydrogen atoms and the shortness of the OH bonds, water is among the nonlinear triatomic molecules displaying the largest rotational constants. For that reason, a large vibration-rotation interaction arises leading to an arduous ro-vibrational energy level calculation. In the present paper, an overview of the various methods which have been developed for the calculation of the water molecule spectrum will be given and their accuracies will be compared. Special emphasis will be given to the newly developed Bending-Rotation Hamiltonian approach and the results obtained when using this formalism to build a database for the water molecule will be examined.

## Line Parameters for Water in the Thermal Infrared

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We describe results of recent experiments on the broadening of room-temperature water transitions by nitrogen in the 400-600  $\text{cm}^{-1}$  range. We are in the process of incorporating these and other results into a comprehensive model of collision-broadening in this region.

## Consensus Assignments for Water-Vapor Lines not Assigned in HITRAN 13,200 to 16,500 $\text{cm}^{-1}$

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There are nearly 800 water-vapor lines in the 13200-16500  $\text{cm}^{-1}$  region that do not have ro-vibrational assignments in the HITRAN database. The positions and intensities in the database were determined by Mandin et al<sup>1</sup> but assignments could not be determined at that time. Polyansky et al<sup>2</sup> have now assigned over 600 of the unassigned lines in the 13200-16500  $\text{cm}^{-1}$  region. Schwenke<sup>3</sup> has also given ro-vibrational assignments to many of these unassigned lines throughout the visible and near-infrared. Both articles change the assignments of some HITRAN lines. Carleer et al<sup>4</sup> extend assignments to some weaker lines measured by them on new spectra with excellent signal/noise. However, some lines measured by Mandin et al<sup>1</sup> were omitted by Carleer et al<sup>4</sup> because of blends due to lower spectral resolution. The ro-vibrational assignments of Polyansky et al<sup>2</sup> completely agree with those in Schwenke's article for only about 200 lines. However, Schwenke's *ab initio* line list is available on his internet site (<http://ccf.arc.nasa.gov/dschwenke>). A detailed comparison of the Polyansky et al<sup>2</sup> line list, the Carleer et al<sup>4</sup> line list, and the Schwenke *ab initio* line list shows a larger number of agreements. In many cases, the disagreement is only about the vibrational and/or rotational upper level, while there is agreement on the lower state assignment and energy level,  $E''$ , which is of primary importance for atmospheric applications. We will present a line list of consensus assignments in the 13200-16500  $\text{cm}^{-1}$  region for consideration of inclusion on the HITRAN and GEISA databases. This will substantially reduce the number of unassigned lines in the databases in this spectral region.

1. J.-Y. Mandin et al, *J. Mol. Spectrosc.* **116**, 167-190 (1986).

2. O. Polyansky et al, *J. Mol. Spectrosc.* **189**, 291-300 (1998).

3. D.W. Schwenke, *J. Mol. Spectrosc.* **190**, 397-402 (1998).

4. M. Carleer et al, *J. Chem. Phys.* **111**, 2444-2450 (19xx).

## The Care and Feeding of Databases

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It now seems fairly clear that most of the submissions of molecular parameters to the HITRAN database are produced by workers who are somewhat more interested in molecular analysis than in accurate database numbers (at least in the case of H<sub>2</sub>O, which is the basis for all of my remarks). This is borne out by the fact that the resulting compilation is usually a poor representation of the data from which it was derived. Examples will be shown to illustrate this point. In an era when great sums of money are being spent to identify new sources of absorbance in the atmosphere, it would seem prudent to first straighten out one of the major sources of that absorbance. Some suggestions will be offered for modest (some even painless) but useful changes to the database format, and there will be some discussion of the steps needed to ensure an accurate comparison between derived parameters and the raw data from which they came.

## Experimental Study of Self- and Air-broadened Water Vapor Lines

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Line positions, line strengths, self- and air-broadening coefficients, self- and air-pressure-induced frequency-shifts, temperature-dependences of air-broadening coefficients of water vapor were obtained with a Bruker IFS120 Fourier-transform spectrometer in the spectral regions  $950\text{--}2067\text{ cm}^{-1}$  and  $3600\text{--}4050\text{ cm}^{-1}$ . Two short cryogenically-cooled stainless cells with path lengths of 9.28 and 2.15 cm were used for the study of the very strong lines in these regions. For the weak lines in the spectral region  $950\text{--}1300\text{ cm}^{-1}$ , a multiple-reflection White cell was used. The White cell was adjusted for pathlengths between 3.2 and 41.6 m in increasing steps of 3.2 m. A global non-linear least-square fitting algorithm was developed for the retrieval of the parameters. Careful consideration was given to the determination of the appropriate instrumental function. The results have been compared with previous studies.

**Laboratory Spectroscopy to Support EOS:  
Water Line Parameters near 0.94  $\mu\text{m}$  (940 nm) for SAGE III**

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For atmospheric applications, over 3000 line positions and intensities of water have been remeasured by least-squares curve-fitting of 17 water spectra that cover three orders of magnitude of intensity. In addition, using 9 spectra of air + water mixtures, over 500 air-broadened Lorentz widths and 450 pressure-induced shifts in positions have been obtained primarily for the strongest transitions of three parallel vibrational bands (121), (201) and (003). All data have been recorded at resolutions of 0.012 and 0.021  $\text{cm}^{-1}$  using the Fourier-transform spectrometer located at Kitt Peak. Comparisons with previous studies will be made, and the rotation-vibration dependences of the broadening coefficients will be discussed.

## Weak Lines in the Water Vapour Near-infrared and Visible Spectrum

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New measurements and theoretical calculations of the near-infrared and visible spectrum of water vapour are summarized. A significant improvement of the signal-to-noise ratio (S/N) by approximately a factor 7.5 in the spectral region  $9500\text{-}16000\text{ cm}^{-1}$  compared to the spectra underlying the HITRAN96 database in this region lead to a large number of previously unknown weak lines in the water spectrum. The new measurements achieved a S/N of up to 5000:1 at an absorption pathlength of  $l = 800.75\text{m}$ . A recent extension of the study yielding measurements in the near-infrared ( $6500\text{-}10500\text{ cm}^{-1}$ ,  $l = 480.75\text{m}$ ) will also be reported. The assignment of the new lines based on theoretical calculations using *ab initio* methods will be discussed. The effect of the large number of weak lines on the energy absorbed by a clear-sky atmosphere will be evaluated and may highlight the importance of an upgrade of the existing database.

## New Studies of the Visible and Near-Infrared Absorption by Water Vapour and some Problems with HITRAN

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New measurements and theoretical calculations of integrated line intensities of water-vapour bands in the visible and the near-IR are summarised. Two different methods of experimental data reduction were used and the results compared with *ab initio* and empirically adjusted *ab initio* theory and with the archived spectra that were used to generate the current HITRAN database for water. Systematic differences of between 5 and 35%, depending on the band under discussion, are found for the ratio of new data to that given in HITRAN-96. These differences are not removed by the recent correction to the HITRAN-96 database.<sup>1</sup> The new data will substantially increase the calculated absorption of solar energy in climate models by a moist cloud-free atmosphere.

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1. L.P. Giver et al, *J. Quant. Spectrosc. Radiat. Transfer* **66**, 101-105 (2000).

## AUTHOR INDEX

|          |   |          |   |
|----------|---|----------|---|
| <b>A</b> | <p>Arcas, P. .... 30</p>  | <b>G</b> | <p>Gamache, R. R. .... 11, 31<br/>           Gille, J. C. .... 21<br/>           Giver, L. P. .... 31, 43, 55<br/>           Glatthor, N. .... 8, 23<br/>           Godoy, C. .... 52<br/>           Goldman, A. .... 11, 12, 21, 31, 39, 42<br/>           Guelachvili, G. .... 44</p> |
| <b>B</b> | <p>Ballard, J. .... 21<br/>           Belmiloud, D. .... 59, 60<br/>           Benner, D. C. .... 32, 37, 38<br/>           Birk, M. .... 29, 48<br/>           Bogumil, K. .... 6<br/>           Brault, J. W. .... 43, 56, 59, 60<br/>           Brown, A. .... 14<br/>           Brown, L. R. .... 37, 38, 41, 43, 58<br/>           Burger, H. .... 47<br/>           Burrows, J. P. .... 6, 39</p>   | <b>H</b> | <p>Hannigan, J. W. .... 42<br/>           Hermans, C. .... 7<br/>           Himmelmann, S. .... 39<br/>           Höpfner, M. .... 24</p>   |
| <b>C</b> | <p>Camy-Peyret, C. .... 30<br/>           Canas, A. A. D. .... 59<br/>           Carleer, M. R. .... 7<br/>           Chackerian, C. .... 43, 55<br/>           Chance, K. .... 16, 17, 19, 42<br/>           Chédin, A. .... 4<br/>           Cheung, A. S-C. .... 50, 51<br/>           Chursin, A. .... 4<br/>           Claveau, C. .... 45<br/>           Coffey, M. T. .... 42<br/>           Cohen, E. A. .... 27<br/>           Colin, R. .... 7<br/>           Cottaz, C. .... 41<br/>           Coudert, L. H. .... 53<br/>           Cox, G. .... 50<br/>           Coyote, S. .... 10</p> | <b>I</b> | <p>Imajo, T. .... 50<br/>           Ito, K. .... 49, 50</p>   |
| <b>D</b> | <p>Dana, V. .... 44, 45<br/>           Devi, V. M. .... 32, 37, 38<br/>           Donahue, N. M. .... 54<br/>           Drouin, B. J. .... 27</p>   | <b>J</b> | <p>Jacob, D. J. .... 17<br/>           Jacquemart, D. .... 44, 45<br/>           Jacquinet-Husson, N. .... 4<br/>           Jamieson, M. J. .... 51<br/>           Jenouvrier, A. .... 7<br/>           Johnson, D. J. .... 16<br/>           Jucks, K. W. .... 16</p>                  |
| <b>E</b> | <p>Edwards, D. P. .... 21<br/>           Esmond, J. R. .... 49, 50</p>  | <b>K</b> | <p>Kellmann, S. .... 8<br/>           Killinger, D. K. .... 26<br/>           Kleffmann, J. .... 47<br/>           Kleiner, I. .... 33, 41<br/>           Kromminga, H. .... 6<br/>           Kurosu, T. P. .... 17, 19</p>   |
| <b>F</b> | <p>Fally, S. .... 7<br/>           Flaud, J.-M. .... 2, 29, 30, 39, 47<br/>           Fleischmann, O. C. .... 6<br/>           Fraser, G. T. .... 13<br/>           Freedman, R. S. .... 43, 55<br/>           Funke, B. .... 23</p>  | <b>L</b> | <p>Lafferty, W. J. .... 13<br/>           Learner, R. C. M. .... 50, 59, 60<br/>           Lees, R. M. .... 34<br/>           Leung, K. W-S. .... 50<br/>           Lo, D. H-Y. .... 50<br/>           Lopez-Puertas, M. .... 23<br/>           Lugez, C. L. .... 13</p>                |
|          |   | <b>M</b> | <p>Ma, Q. .... 15<br/>           Mandin, J.-Y. .... 31, 44, 45<br/>           Mankin, W. G. .... 42<br/>           Martin, R. V. .... 17</p>  |

|                      |        |
|----------------------|--------|
| Martin-Torres, F. J. | 23     |
| Massie, S. T.        | 12, 21 |
| Maté, B.             | 13     |
| Matsui, T.           | 49, 50 |
| McCarthy, M. C.      | 3      |
| Mérianne, M.-F.      | 7      |
| Miller, C. E.        | 27     |
| Müller, H. S. P.     | 27     |
| Murcay, F. J.        | 31     |
| Murray, J. E.        | 50     |

## N

|                |    |
|----------------|----|
| Nakajima, H.   | 20 |
| Neshyba, S.    | 18 |
| Newnham, D. A. | 60 |

## O

|            |       |
|------------|-------|
| Orphal, J. | 6, 39 |
|------------|-------|

## P

|                  |        |
|------------------|--------|
| Palmer, P. I.    | 17     |
| Parkinson, W. H. | 49, 50 |
| Pawelke, G.      | 47     |
| Perrin, A.       | 30, 39 |
| Picqué, N.       | 44     |
| Polyansky, O. L. | 59     |
| Predoi-Cross, A. | 37     |

## R

|                 |            |
|-----------------|------------|
| Reuter, D. C.   | 54         |
| Rinsland, C. P. | 31, 39, 42 |
| Rothman, L. S.  | 1, 9, 31   |

## S

|                 |        |
|-----------------|--------|
| Sams, R. L.     | 38     |
| Sasano, Y.      | 19, 20 |
| Schermaul, R.   | 59, 60 |
| Schreier, F.    | 29     |
| Schrijver, H.   | 25     |
| Schroeder, J.   | 9      |
| Schwenke, D. W. | 55     |
| Scott, N.       | 4      |
| Sirota, J. M.   | 54     |
| Smith, K.       | 60     |
| Smith, M. A. H. | 32, 38 |
| Solodov, A. M.  | 13     |

|                 |        |
|-----------------|--------|
| Spietz, P.      | 6      |
| Spurr, R. J. D. | 17     |
| Stephen, T. M.  | 31, 39 |
| Steyert, D. W.  | 54     |
| Stiller, G. P.  | 8, 23  |
| Sugita, T.      | 20     |
| Sun, C.         | 46, 57 |

## T

|                |        |
|----------------|--------|
| Tarrago, G.    | 41     |
| Tennyson, J.   | 59, 60 |
| Thaddeus, P.   | 3      |
| Thorne, A. P.  | 50     |
| Tipping, R. H. | 14, 15 |
| Tjemkes, S. A. | 22     |
| Tong, G. S-M.  | 51     |
| Toth, R. A.    | 37, 58 |
| Traub, W. A.   | 16     |

## V

|                   |                |
|-------------------|----------------|
| Valentin, A.      | 30             |
| Vandaele, A.-C.   | 7              |
| Vander Auwera, J. | 47             |
| Varanasi, P.      | 36, 46, 55, 57 |
| Vázquez, G. J.    | 52             |
| Voigt, S.         | 6, 39          |

## W

|            |        |
|------------|--------|
| Wagner, G. | 29, 48 |
| Wang, W.   | 54     |

## X

|           |    |
|-----------|----|
| Xu, L.-H. | 34 |
|-----------|----|

## Y

|              |        |
|--------------|--------|
| Yokota, T.   | 19, 20 |
| Yoshino, K.  | 49, 50 |
| Young, E. F. | 10     |

## Z

|                |        |
|----------------|--------|
| Zimmermann, A. | 24     |
| Zobov, N. F.   | 60     |
| Zou, Q.        | 46, 57 |