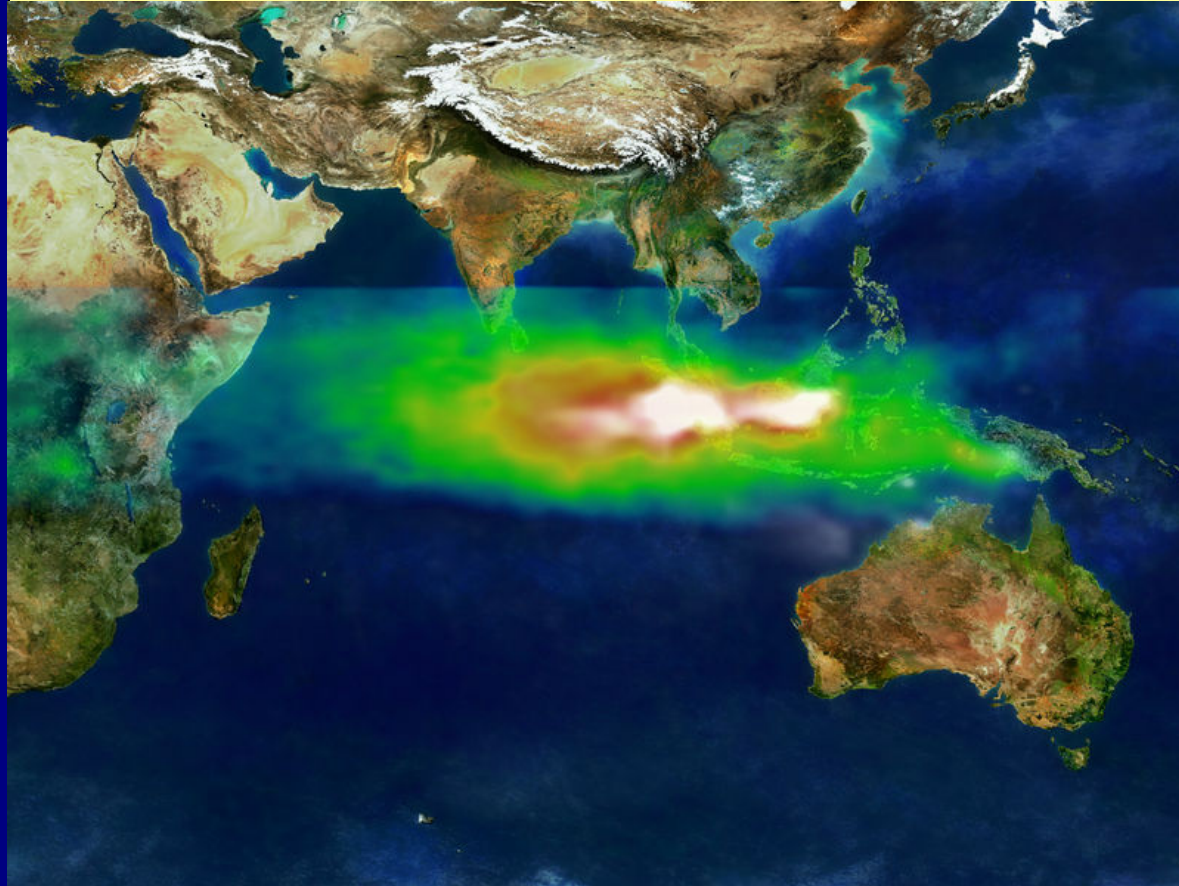


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**The 10th HITRAN
Database Conference**

2008

June 22 – June 24, 2008

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Front page: This image shows the pollution over Indonesia and the Indian Ocean on October 22, 1997. White represents the aerosols (smoke) that remained in the vicinity of the fires. Green, yellow, and red pixels represent increasing amounts of tropospheric ozone (smog) being carried to the west by high-altitude winds. Researchers tracked the pollution using data from NASA's Earth Probe Total Ozone Mapping Spectrometer (TOMS) satellite instrument.

The HITRAN Project has been funded by grants from the National Aeronautics and Space Administration.

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SESSION I: Astrophysics

I-1. High-Resolution Spectroscopy and Astronomical Detection of Molecular Anions

Sandra Brünken, Carl A. Gottlieb, Harshal Gupta¹, Michael C. McCarthy,
and Patrick Thaddeus

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The importance of negative ions (anions) in astronomy was demonstrated in 1939 by Rupert Wildt who showed that H^- is the major source of optical opacity in the solar atmosphere, and therefore the material which one mainly sees when looking at the sun and similar stars. It is remarkable that in the many years since, during which nearly 130 neutral molecules and 14 positive molecular ions have been found in a variety of astronomical sources, no molecular anion had been identified, owing in large part to the absence of laboratory rotational spectra.

This puzzle has been solved with our recent laboratory identification of the large molecular anion C_6H^- as the carrier of a series of unidentified rotational emission lines in the circumstellar shell of the late carbon star IRC+10216, and its detection in the cold molecular cloud TMC-1². Since then, high resolution spectroscopy of molecular anions and searches for them in astronomical sources is advancing at an astonishing pace. Five additional, closely related carbon chain anions (CCH^- , C_4H^- , C_8H^- , CN^- , and C_3N^-) were in the last year detected in our laboratory, and three of them have in the meantime also been detected with surprisingly high abundances in space using highly sensitive radio telescopes³.

In this talk I will briefly describe the spectroscopic techniques that we use to detect and characterize molecular radicals and ions via their high-resolution gas-phase spectra, and how these data can be used to identify these molecules in astronomical sources. I will then summarize the recent results on molecular anions in detail and outline how these new findings might improve our knowledge about the interstellar and circumstellar medium.

¹also at: Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, The University of Texas, Austin, TX 78712, USA

²M. C. McCarthy, C. A. Gottlieb, H. Gupta, and P. Thaddeus, *ApJL* 652 (2006), L141.

³H. Gupta, S. Brünken, F. Tamassia, C. A. Gottlieb, M. C. McCarthy, and P. Thaddeus, *ApJL* 655 (2007) L57; S. Brünken, C. A. Gottlieb, H. Gupta, M. C. McCarthy, and P. Thaddeus, *A&A* 464 (2007) L33; J. Cernicharo, M. Guelin, M. Agundez, K. Kawaguchi, M. C. McCarthy, and P. Thaddeus, *A&A* 467 (2007) L37; S. Brünken, H. Gupta, C. A. Gottlieb, M. C. McCarthy, and P. Thaddeus, *ApJL* 664 (2007) L43; C. A. Gottlieb, S. Brünken, M. C. McCarthy, and P. Thaddeus, *JCP* 126 (2007) 191101; P. Thaddeus, C. A. Gottlieb, H. Gupta, S. Brünken, M. C. McCarthy, P. Thaddeus, M. Agundez, M. Guelin, and J. Cernicharo, *ApJ* 677 (2008) 1132; N. Sakai, T. Sakai, Y. Osamura, and S. Yamamoto, *ApJL* 667 (2007) L65; N. Sakai, T. Sakai, and S. Yamamoto, *ApJL* 673 (2008) L71; M. Agundez, J. Cernicharo, M. Guelin, M. Gerin, M. C. McCarthy, and P. Thaddeus, *A&A* 478 (2008) L19.

I-2. Characterizing Pale Blue Dots in the Sky - Spectral Fingerprints from Earth to Super-Earth

Lisa Kaltenegger

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There are many puzzle-pieces to assemble if we want to detect life, signs of life, or even conditions for life, on rocky exoplanets. What detectable signatures does life leave in a planetary atmosphere or on a planetary surface and what does HITRAN have to do with it? Future space missions will provide the pieces to solve this puzzle. In this talk we will look at the evidence that we are searching for, as well as what we are likely to get, and the challenges we face to define these pieces.

I-3. Precise Modeling of Atmospheric Absorption Features in High-Resolution Astronomical Spectra

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We present the latest results in modeling atmospheric absorption features in high-resolution astronomical spectra, both, in the optical and near infrared at spectral resolutions of $R=30,000 - 100,000$.

By using a variety of meteorological input parameters to build realistic atmospheric profiles and by modeling the instrumental profile of our spectrographs, we achieve a fit to telluric lines at the 1% level. While this is often sufficient for the removal of such lines from stellar spectra, we outline the range for further improvements and identify the most likely reasons for the current limitations.

We will further emphasize the prospects for using telluric lines as a restframe for precise radial velocity measurements in the near infrared, which may facilitate the detection of very low mass extrasolar planets around late type stars and brown dwarfs. Finally, we will give an outlook how telluric features in astronomical spectra may be used for monitoring climate changes by precise measurements of the column density of CO_2 and CH_4 .

I-4. High-Accuracy Spectral Lines for Radiation Transport in Stellar Atmospheres

**Amit R. Sharma,^a Bastiaan J. Braams,^a Joel M. Bowman,^a
Robert Warmbier,^b Ralf Schneider,^b and Peter H. Hauschildt^c**

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The theory of radiative transfer is an important element for the understanding of the spectral signature and physical structure of stellar atmosphere. PHOENIX¹ is a such, very general non-Local Thermodynamic Equilibrium (NLTE) stellar atmosphere computer code which can handle very large model atoms/molecules as well as line blanketing by hundreds of millions of atomic and molecular lines. The code is used to compute model atmospheres and synthetic spectra (solution of the radiative transport equations) for, e.g., novae, supernovae, M and brown dwarfs, O to M giants, white dwarfs and accretion disks in Active Galactic Nuclei (AGN). The radiative transfer in PHOENIX is solved in spherical geometry and includes the effects of special relativity (including advection and aberration) in the modeling. The code includes a large number of NLTE and LTE background spectral lines and solves transport equation for each of the lines. The numerical solution requires many wavelength points which arise in the non-LTE case by balancing all populating and de-populating processes from each molecular level (typically 150,000 to 300,000 points). Typically, HITRAN and GEISA are the computer accessible spectroscopic databases used by such transport codes. However, these spectroscopic databases are far from adequate and complete and there is constant demand for more complete and consistent spectral lines for the existing and newly observed molecules in space.

We used the code MULTIMODE² to obtain eigenvalues and eigenfunctions of the general so-called Watson Hamiltonian using variational methods. The procedure begins with a Hartree form for the wavefunction and then vibrational self-consistent field (VSCF) equations are solved for the given state (usually the ground vibrational state) The Hartree form for the wavefunction in the VSCF method is the representation of the vibrational wavefunction as a product of single-mode wavefunctions. From the converged single mode Hamiltonians a basis of virtual states is obtained and these are used in subsequent virtual space CI calculations. This is very much in the spirit of CI approaches taken in electronic structure theory. The application of this methodology for molecules

¹P. H. Hauschildt *J. Quant. Spect. Rad. Tran.* **50**(3),301-318, Sep 1993.

²J. M. Bowman *Int. Rev. Phys. Chem.* **22**(3),608-610, 2003.

with more than 4 atoms is made possible by the so-called n-mode representation of the potential³ VSCF method augmented by CI or perturbation theory results in improved vibrational frequencies. These methods can accurately solve the problem of coupled vibrations, which physically arise because the vibrationally excited states of polyatomic molecules exhibit displacements, so large that anharmonicities become important, causing the harmonic modes to mix. Following the (ro-)vibrational state calculations we compute Einstein coefficients and spectral intensities for all allowed transitions. However, a stringent requirement for these calculations is a highly accurate potential energy surface.

Ab initio-based, full-dimensional potential energy surfaces (PES) are employed in this work. These potentials are global fits to of the order of 10^4 electronic energies using a basis of polynomials in Morse-like functions of all the internuclear distances. The polynomial basis is invariant with respect to all permutations of like atoms and, as a result, yield highly compact and accurate representations of the PES. Similar techniques are also employed to represent the dipole moment surface (DMS)⁴ for a polyatomic molecules in the normal coordinate space using full dimensional permutationally invariant potential energy surface. The VSCF, VCI and PES generation scheme, together, can consistently deliver high accuracy spectral lines for large number of molecules for radiation transport application in astrophysics.

Chemically interesting singlet carbocation $C_2H_5^+$, known as the ethyl cation, is of special interest in the field astrophysics, specially in the ionosphere of Titan, due to the recent observations by cassini spacecraft. Ethyl cation exhibits interesting structural minimum and transition state, namely the bridged structure (or non-classical) and the Y-shape (or classical) structure. The calculations performed at the Hartree-Fock level of theory found the classical form to be a real minimum and the bridged structure to be less stable than the classical form. However, as soon as correlation effects are taken into account the classical form turns out to be a first order saddle point and less stable than the non-classical form. In the lower-lying structure, referred to as the “bridged” structure (or non-classical structure), one hydrogen forms a bridge with the two carbon nuclei and the other four hydrogen atoms (two hydrogen on each carbon nuclei) are nearly co-planar with the two carbon atoms. Semi-global potential energy surface is developed using the method described above with the electronic structure energy calculated using the fourth order MØLLER-PLESSET (MP4) perturbation theory with contributions due to single, double, triple and quadruple excitations to the electron correlation energy(MP4(SDTQ)). The dipole moment surface is calculated at the MP2 level of theory. Multimode code is used to calculate the vibrational energies up to 4000 cm^{-1} . Zero point vibrational energy is further compared with Diffusion Monte Carlo (DMC) calculations. The other most interesting and extensively studied molecule is

³S. Carter, C. J. Culik and J. M. Bowman *J. Chem. Phys.* **107**(24),10458-10469, 1997.

⁴X. Huang, B. J. Braams and J. M. Bowman *J. Chem. Phys.* **122**,044308, 2005.

methane. Adiabatic rotation approximation is used to obtain Hamiltonian for rotating molecule. Ro-vibrational energies, transition matrix elements and Einstein coefficients are calculated for $J = 0, 1, 3, 5, 10, 15, 20, 25, 30$. The present calculations are in good agreement with the well established HITRAN database for methane.

I-5. Non-linear Effects of Atmospheric Extinction on Observations in Astronomy

Frédéric Zagury

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I have studied the modifications of the spectrum in the immediate vicinity of a star, due to the interaction (diffraction and scattering) between starlight and the atmosphere. Additionally I have considered the dependence of atmospheric extinction on the kind of celestial object which is observed. The atmosphere seems to have a much stronger effect on faint extended objects (nebulae, galaxies) than it has on bright stars in the blue (shortward of 6500 Å). This questions the traditional data-reduction process used in astronomy and suggests that unexpected limitations on astronomical observations from Earth might occur, especially for the deep observations planned with the next generation of large telescopes.

I will show the role of absorption by the main atmospheric molecules in these non-linear effects of atmospheric extinction, and emphasize the implications they might have for some important issues in Astronomy, and for the small scale structure of the atmosphere.

Finally, the results presented here suggest that modern high resolution (spectral and spatial) means of observation used in Astronomy may be of interest for the study of the atmosphere.

SESSION II: Databases

II-1. Near-Infrared Carbon Dioxide Spectral Database

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A new spectroscopic database for carbon dioxide in the near infrared is presented to support remote sensing of the terrestrial planets (Mars, Venus and the Earth). The compilation contains over 28,500 transitions of 213 bands from 4300 to 7000 cm^{-1} and involves nine isotopologues: $^{16}\text{O}^{12}\text{C}^{16}\text{O}$ (626), $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ (636), $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ (628), $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ (627), $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ (638), $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ (637), $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ (828), $^{17}\text{O}^{12}\text{C}^{18}\text{O}$ (728), and $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ (838). Calculated line positions, line intensities, Lorentz half width and pressure-induced shift coefficients for self and air broadening are taken from our recent measurements and are presented for the Voigt molecular line shape. The database includes line intensities for 153 bands measured using the McMath-Pierce Fourier transform spectrometer at the Kitt Peak National Solar Observatory. The available broadening parameters (half widths and pressure-induced shifts) of $^{16}\text{O}^{12}\text{C}^{16}\text{O}$ are applied to all isotopologues. Broadening coefficients are computed using empirical expressions that have been fitted to the experimental data. The line intensities included in the catalog vary from 4×10^{-30} to 1.29×10^{-21} $\text{cm}^{-1}/(\text{molecule cm}^{-2})$ at 296 K.

The research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology and the College of William and Mary, under contracts and cooperative agreements with the National Aeronautics and Space Administration.

II-2. High Sensitivity CW-CRDS Spectroscopy of the Eight Most Abundant CO₂ isotopologues between 5851 and 7045 cm⁻¹. Critical Review of the Current Databases

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The exhaustive line positions analysis of the absorption spectrum of carbon dioxide in natural abundance has been performed on the basis of high sensitivity CW-Cavity Ring Down spectroscopy between 5851 and 7045 cm⁻¹ (1.71-1.42 μm). The achieved sensitivity (noise equivalent absorption $\alpha_{min} \sim 2 - 5 \times 10^{-10}$ cm⁻¹) combined with the high linearity and dynamics (more than 4 decades) of the CW-CRDS technique, have allowed the detection of 8293 transitions of the ¹²C¹⁶O₂, ¹⁶O¹²C¹⁷O and ¹⁶O¹²C¹⁸O isotopologues. They belong to a total of 130 bands. Line intensities of the weakest transitions are on the order of 2×10^{-29} cm⁻¹/(molecule cm⁻²). The rovibrational assignments were performed on the basis of accurate predictions of the effective Hamiltonian model of the respective isotopologues. The band-by-band analysis has allowed deriving accurate spectroscopic parameters of 121 bands from a fit of the measured line positions. A number of resonance interactions were identified. In particular, the first observation of an interpolyad coupling is reported for the ¹⁶O¹²C¹⁸O isotopologue.

A similar experimental database has been constructed for the ¹³C¹⁶O₂, ¹⁶O¹³C¹⁸O, ¹⁶O¹³C¹⁷O, ¹³C¹⁸O₂ and ¹⁷O¹³C¹⁸O isotopologues of carbon dioxide on the basis of CW-CRDS spectra of carbon dioxide with 99 % enrichment in ¹³C. A total of 8639 transitions of the five ¹³C isotopologues were assigned. They belong to a total of 150 bands while less than 20 bands were previously reported by Fourier Transform spectroscopy in the region. Accurate line intensities of 2039 transitions ranging between 1.1×10^{-28} and 1.3×10^{-23} cm⁻¹/(molecule cm⁻²) were used together with FTS data to determine the effective dipole moment parameters in the frame of the effective operators approach. A list of ¹³C 8639 transitions has been constructed: line positions are experimental values (typical uncertainty on the order of 1×10^{-3} cm⁻¹) while line strengths were calculated at 296 K by using the effective operators approach (typical uncertainty on the order of 5 %). In the case of the ¹³C¹⁶O₂ isotopologue, the reported transitions represent 99.65 % of the total absorbance in the region considered. The obtained experimental datasets

which are the most complete in the considered region, have been used for a critical review of the most currently used spectroscopic databases of carbon dioxide: HITRAN, GEISA, HITEMP, and the recent JPL and CDSO databases.

II-3. CDSD-296 (Carbon Dioxide Spectroscopic Databank): Updated and Enlarged Version for Atmospheric Applications

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We present the current version of the CDSD databank¹ aimed at atmospheric applications. The databank contains line parameters (positions, intensities as well as HITRAN air- and self-broadened halfwidths and coefficients of temperature dependence of air-broadened halfwidths) of eight most abundant isotopic species of CO₂. The reference temperature is 296 K, the intensity cutoff is 10-30 cm⁻¹/(molecule cm⁻²) and the spectral range is 405-12784 cm⁻¹. The databank was generated within the framework of the method of effective operators and based on global fittings of parameters of the effective operator models to observed data collected from the literature. Detailed comparisons with HITRAN and a recent CO₂ databank by Toth² will also be given.

¹S.A. Tashkun, V.I. Perevalov, J-L. Teffo, A.D. Bykov, N.N. Lavrentieva, CDSD-1000, the high-temperature carbon dioxide spectroscopic databank, JQSRT, 82, 165-196, (2003)

²R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, D.Chris Benner, Spectroscopic database of CO₂ line parameters: 4300-7000 cm⁻¹, JQSRT, in press

II-4. Half-Widths and Line Shifts for Transitions in the ν_3 Band of Methane in the 2726 – 3200 cm^{-1} Spectral Region for Atmospheric Applications

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Methane, like CO_2 , is present in the terrestrial atmosphere in trace amounts, but these greenhouse gases are thought to be major drivers of climate change and global warming. To understand these processes and predict the future condition if the atmosphere, scientists utilize global climate models, for which the concentrations of the greenhouse gases are part of the input. In this paper the focus is on methane, for which the vibration-rotation bands between 9 and 1.6 μm are commonly used to monitor concentrations. A major component in the error budget of atmospheric retrievals for methane in the lower troposphere arise from the poor accuracies of the pressure broadening coefficients.

The main source of spectroscopic line parameters for methane is the HITRAN database. The 2004 HITRAN database contains some 251 440 methane transitions. Considering vibration-rotation bands of $^{12}\text{CH}_4$ between 9 and 1.6 μm with the sum of line intensities greater than $10^{-20} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ yields a list of over one hundred thousand transitions. While it is not practical to measure or calculate the line parameters for all transitions, data are needed at least for the strong vibrational bands. Here, we focus on the region 2726 to 3200 cm^{-1} , which still contains over twenty five thousand transitions for $^{12}\text{CH}_4$. The dominant band in this region is the ν_3 band centered at 3018 cm^{-1} .

In this work, Complex Robert-Bonamy calculations of the pressure-broadened half-width and the pressure induced line shift are made for some four thousand transitions in the ν_3 band of methane with N_2 , O_2 , and air as the perturbing gases. This work focuses on A and F symmetry transitions in the spectral range 2726 to 3200 cm^{-1} . More work is needed on the intermolecular potential before calculations can be made for the E-symmetry transitions. The calculations are made at 225 and 296K in order to determine the temperature dependence of the half-width. The calculations are compared with measurements. These data are to support remote sensing of the Earth and Titan atmospheres.

II-5. New Line Parameters for Near-IR Methane and the Oxygen A-Band

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Recent and ongoing studies by various groups will be described for near-IR methane and the oxygen A-band in the context of changes for the HITRAN 2008 database. For methane, a new global analysis of the bands of the main isotope ¹ will permit a total replacement of the calculated positions and intensities up to 4800 cm⁻¹. A few improvements are also available near 6000 cm⁻¹. Probable revisions in methane broadening parameters throughout the infrared will also be detailed. For the oxygen A-band at 13122 cm⁻¹, new studies will provide better accuracies for line positions and intensities of the three most abundant isotopologues. Recent studies demonstrate that non-Voigt molecular line shapes are required to characterize the oxygen A-band in atmospheric spectra, and the choice of broadening parameters will depend on which line shape model is used. Recommendations for future studies of these two molecules will be included.

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

¹Albert et al. (submitted)

Poster Session 1

PI-1. Pressure Broadening Coefficients of the Water Vapor Lines in the Terahertz Region

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We have measured air-broadened coefficients of water vapor in the range of 0.5 to 5 THz using terahertz time-domain spectroscopy and Fourier transform spectroscopy. We have also carried out radiative transfer calculations to demonstrate the changes in wave propagation modeling due to newly measured pressure broadening parameters.

PI-2. Comparison of Measured and Modeled Transmittances in Near-Infrared and Visible Water Vapor Bands

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Absorption of solar radiation by the atmosphere is a critical component of the energy balance of the Earth and a key factor in the evolution of its climate. Water vapor is responsible for much of this absorption due to its abundance and the extended spectral domain over which it is radiatively active. Accurate descriptions of water vapor line and continuum absorption, the underpinnings of radiative transfer models, are thus necessary for accurate global climate model calculations. The comparison of ground-based spectral measurements and radiative transfer model calculations is an effective method for evaluating model calculations of the solar irradiance absorbed in the atmosphere. This work presents comparisons between direct-beam transmittances obtained from the medium-resolution Rotating Shadowband Spectroradiometer (RSS) and corresponding calculations performed by the Code for High Resolution Accelerated Radiative Transfer (CHARTS); the spectral line parameters are obtained from HITRAN 2004 with updates through 2007. The RSS provides spectrally resolved direct-normal irradiances between 360 and 1050 nm, from which the atmospheric transmittance is derived. The comparisons are used to evaluate the accuracy and mutual inter-band consistency of water vapor line parameters in three adjacent water vapor bands centered at 720 nm, 820 nm, and 940 nm. The RSS is deployed at the Atmospheric Radiation Measurement Program's Southern Great Plains Climate Research Facility. Radiosondes, launched every 6 hours, and precipitable water vapor retrieved from two-channel microwave-radiometer measurements (23.8 and 31.4 GHz) are used as input to the radiative transfer model; numerous cases are examined spanning a wide range of precipitable water vapor, sonde-based water vapor profiles, and solar zenith angles.

PI-3. Air-Broadened Halfwidths of the 22 GHz and 183 GHz Water Vapor Lines

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We present a determination of air-broadened half widths of the 22 and 183 GHz water vapor lines and associated uncertainties using comparisons between ground-based radiometric measurements from Atmospheric Radiation Measurement (ARM) sites in Oklahoma and Alaska and MonoRTM, a radiative transfer model. Values of the widths obtained using the measurements are $0.0900 \text{ cm}^{-1}/\text{atm}$ with 1.5 % uncertainty for the 22 GHz line and $0.0992 \text{ cm}^{-1}/\text{atm}$ with 2 % uncertainty for the 183 GHz line. In addition, we present spectroscopic parameters for these lines from new calculations performed using the complex implementation of the Robert-Bonamy theory (CRB). The CRB values of the air-broadened widths are $0.0913 \text{ cm}^{-1}/\text{atm}$ with 3 % uncertainty and a temperature exponent of 0.755 for the 22 GHz line and $0.0997 \text{ cm}^{-1}/\text{atm}$ with 3 % uncertainty and a temperature exponent of 0.769 for the 183 GHz line. We conclude that the values for the air-broadened half widths derived from the measurement/model comparisons show good agreement with the new CRB calculations. For future versions of MonoRTM we will adopt width values of $0.0900 \text{ cm}^{-1}/\text{atm}$ and $0.0997 \text{ cm}^{-1}/\text{atm}$ with temperature dependences of 0.76 and 0.77 for the 22 GHz and 183 GHz lines respectively.

PI-4. Experimental and Theoretical Studies of Water-Vapor Continuum Absorption in the THz Region from 0.3 to 2.7 THz

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Experimental results and theoretical calculations of the continuum absorption by water vapor in the far-IR region from 10 to 90 cm^{-1} (0.3 to 2.7 THz) are presented for the temperature range from 293 to 333 K. The contributions to absorbance resulting from structureless $\text{H}_2\text{O-H}_2\text{O}$, $\text{H}_2\text{O-N}_2$ and $\text{H}_2\text{O-O}_2$ continua have been measured over a wide pressure range with a spectral resolution of 0.04 to 0.12 cm^{-1} .^{1 2} The experimental broadband THz technique using Fourier transform spectroscopy and enhanced absorption in a temperature-controlled multipass cell will be presented.³ The resonant water vapor spectrum was modeled using the HITRAN04 data base and VVW lineshape. After subtracting local contributions from the raw absorbance data, the $\text{H}_2\text{O-H}_2\text{O}$ (self), $\text{H}_2\text{O-N}_2$ and $\text{H}_2\text{O-O}_2$ (foreign) continua were derived both by fitting the entire frequency region based on an assumed quadratic frequency dependence and by fitting to each of the THz windows individually. The experimental absorption coefficients and temperature exponents of the foreign-continuum obtained from individual THz windows are compared to theoretical calculations based on the modified Lanczos method.⁴ New high resolution THz measurements of the O_2 and N_2 pressure broadening coefficients of water lines near the 2.5 THz window region will also be discussed.

¹V. B. Podobedov, D. F. Plusquellic K. M. Siegrist, G. T. Fraser, Q. Ma and R. H. Tipping, JQSR Transfer, 109, 458 (2008)

²V. B. Podobedov, D. F. Plusquellic K. M. Siegrist, G. T. Fraser, Q. Ma and R. H. Tipping, J. Mol. Spectro, in press (2008)

³V. B. Podobedov, D. F. Plusquellic and G. T. Fraser, JQSR Transfer 91, 287 (2005)

⁴Q. Ma and R. H. Tipping. J. Chem. Phys. 117, 10581 (2002)

PI-5. H₂O/HDO/D₂O Fourier Transform Infrared Spectroscopy: the 5600-11600 cm⁻¹ Region

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In the continuation of our work dedicated to the spectroscopy of the stable isotopologues of water vapor (H₂¹⁶O, H₂¹⁷O, H₂¹⁸O, HDO, D₂O)^{1 2 3 4}, and considering the current atmospheric and spectroscopic interests for these species (e.g.^{5 6 7 8}, and references therein), this work presents line parameters of H₂O, HDO and D₂O in the 5600-11600 cm⁻¹ region. Long-pathlength (up to 1000 m) Fourier transform absorption spectra of natural H₂O and H₂O:HDO:D₂O mixtures have been recorded at different partial pressures and at room temperature with a BRUKER 120M spectrometer. Spectra in the presence of dry synthetic air were also recorded and usual spectral line parameters are systematically measured. The long path measurements are completed with short path (down to 30 cm) ones registered with the home made GSMA step by step Fourier Transform Spectrometer in order to determine the parameters of the most intense lines that are completely saturated in the long path spectra. The assignment of the lines to the different isotopologues was based on ratios between spectra of different relative abundances and accurate partial pressures were determined from ratios between line areas. The rovibrational assignment of each transition is based on the most recent calculation from the Partridge and Schwenke surfaces. The spectral region between 5600 and 11600 cm⁻¹ has been completely measured. The assignment of the 5600-8800 cm⁻¹ region is under progress whereas it is completed in the upper region. A detailed linelist comprising absolute positions, intensities, self-broadenings and assignments is presented. In the global region more than 25000 lines were measured for the two species HDO and D₂O.

¹A. Jenouvrier et al. *J. Quant. Spectrosc. Radiat. Transfer* **105** (2), 326-355 (2006).

²O. V. Naumenko et al. *J. Mol. Spectrosc.* **238** (1), 79-90 (2006).

³R. N. Tolchenov et al. *J. Mol. Spectrosc.* **233** (1), 68-76 (2005).

⁴M. Bach et al. *J. Mol. Spectrosc.* **232** (2), 341-350 (2005).

⁵M. Schneider et al. *Atmos. Chem. Phys. Discuss.* **5**, 9493-9545 (2005).

⁶H. Brogniez et al. *J. Geophys. Res.* **111**, d21109 (2006).

⁷D. C. Tobin et al. *J. Geophys. Res.* **111**, d09S14 (2006).

⁸L. S. Rothman et al. *J. Quant. Spectrosc. Radiat. Transfer* **96** (2), 139-204 (2005).

Due to the presence of natural ^{18}O , some lines of HD^{18}O are also detected. The results are compared with recent literature data and improvements as well as future needs are briefly discussed.

PI-6. Global Modeling of $^{13}\text{C}^{16}\text{O}_2$ Absolute Line Intensities from CW-CRDS and FTS Measurements in the 1.6 and 2.0 micrometer Regions

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Line intensities of $^{13}\text{C}^{16}\text{O}_2$ have been measured between 5851 and 6580 cm^{-1} using CW-Cavity Ring Down Spectroscopy and in the 4700 – 5050 and 6050 – 6850 cm^{-1} regions using Fourier transform spectroscopy. As a result of the high sensitivity (noise equivalent absorption $\alpha_{\text{min}} = 3 \times 10^{-10} \text{ cm}^{-1}$) and high dynamics allowed by CW-CRDS, accurate line intensities of 2039 transitions ranging between 1.1×10^{-28} and $1.3 \times 10^{-23} \text{ cm}^{-1} / (\text{molecule cm}^{-2})$ were measured with an average accuracy of 4 %. These transitions belong to a total of 48 bands corresponding to the P=9 series of transitions. Additionally, unapodized absorption spectra of ^{13}C -enriched samples have been recorded using a high-resolution Bruker IFS125HR Fourier transform spectrometer. Spectral resolutions of 0.004 cm^{-1} (Maximum Optical Path Difference MOPD = 225 cm) and 0.007 cm^{-1} (MOPD = 128.6 cm), and pressurepath length products in the ranges 5.2-12 hPa m and 69-450 hPa m have been used for the lower and higher energy spectral regions, respectively. Absolute line intensities have been measured in the 2001i – 00001, 3001i – 00001 ($i = 1, 2, 3$) and 00031 – 00001 bands. An excellent agreement was achieved for the line intensities of the 3001i - 00001 ($i = 1, 2, 3$) bands measured by both FTS and CW-CRDS. The CW-CRDS and FTS experimental intensity data together with selected intensity information from the literature have been fitted simultaneously using the effective operators approach. Two sets of the effective dipole moment parameters have thus been obtained, which reproduce the observed line intensities in the 2.0 μm and 1.6 μm regions within experimental uncertainties.

PI-7. Temperature Dependence of Air-Broadened Half Width and Pressure Shift Coefficients in the 30012 – 00001 Band of $^{12}\text{C}^{16}\text{O}_2$

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For atmospheric applications, the temperature dependence of half width and shift coefficients is required on a line-by-line basis. In this study, transitions of carbon dioxide in the 30012 – 00001 band broadened by air were recorded using two different Fourier Transform Spectrometers (A Bomem in Ottawa and the McMath-Pierce FTS in Arizona) using dilute mixtures at temperatures between 215 K and 296 K. These data were analyzed using a multispectrum fit technique applying a Speed Dependent line shape model with line mixing. The positions and intensities of the spectral lines were constrained to conform to the appropriate quantum mechanical relationships reducing the number of parameters extracted from the spectra and reducing correlations between parameters. Pressure broadening coefficients, pressure shifts, their temperature dependencies, line mixing and speed dependence are all retrieved simultaneously in the same solution. The research performed at University of Lethbridge and the National Research Council of Canada was sponsored by the National Sciences and Engineering Research Council under the Strategic Research Program. Part of the research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology and the College of William and Mary, under contracts and cooperative agreements with the National Aeronautics and Space Administration.

PI-8. Analysis of the $^{18}\text{O}_3$ CRDS Spectra in the 6000 – 7000 cm^{-1} Spectral Range: Comparison with $^{16}\text{O}_3$

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During the last two years, we have investigated the high energy levels of the $^{16}\text{O}_3$ molecule¹, and references herein, approaching the dissociation limit ($\approx 8000 \text{ cm}^{-1}$) from high sensitivity CW-CRDS spectra recorded in Grenoble.

The spectra of the totally substituted $^{18}\text{O}_3$ isotopologue have been also recorded in the same 6000 – 7000 cm^{-1} spectral range in order to provide complementary information on the Potential Energy and the Dipole Moment Surfaces.

Up today, 14 bands (10 A-type bands and 4 B-type bands) have been observed and analyzed. We present here the results of the analyses for each band : range of observed quantum numbers, parameters of the effective Hamiltonian and effective transition moment, as well as several comparisons between observed and calculated spectra.

The comparison between the vibrational energies predicted from the potential function and the observed band centers will be discussed for the the $^{18}\text{O}_3$ isotopologue and the $^{16}\text{O}_3$ molecule.

¹A. Campargue, A. Barbe, M.-R. De Backer-Barilly, Vl. G. Tyuterev and S. Kassi, *Phys. Chem. Chem. Phys.*, **10**, 2925-2946, (2008).

PI-9. A Review of the O₃ Absorption Cross Sections in the Orbiting Carbon Observatory O₂-Channel Spectral Region (755-775 nm)

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The Orbiting Carbon Observatory (OCO) is a NASA Earth System Science Pathfinder Project mission to be launched in December 2008. OCO is designed to make precise, time-dependent global measurements of atmospheric carbon dioxide (CO₂) from an Earth orbiting satellite. One of the three OCO channels is located in the 755 – 775 nm spectral region. Observations of the O₂ A-band spectra in this channel will be used to infer the presence of clouds and optically thick aerosols that preclude full column measurements of CO₂. They also will be used to retrieve the total atmospheric pressure, as well as to measure the length of the path of solar light as it passes through the atmosphere. Given the high accuracy requirements of the OCO data products an accurate knowledge of any atmospheric contribution in the OCO channels is needed. The ozone absorption spectrum in the Chappuis-Wulf bands at 760-nm is one of these contributions. These bands are around 10 times smaller and more structured than the Chappuis band near 600-nm and accurate laboratory measurements of their weak absorptions are difficult to achieve due to the large ozone column densities required and, as a result, only a limited number of measurements are available. In this paper a review of 5 existing databases of O₃ absorption cross sections in the 755 – 775 nm spectral region is presented. A comparison of these databases reveals differences that are significantly larger than the reported uncertainties in the reference cross sections themselves. In addition, the ozone cross sections are temperature dependent in the Chappuis-Wulf bands in this region, varying by around 9-11% in the absorption peaks between 298 K and 203 K. The effects of the current uncertainties in the calculation of absorption coefficients in the O₂-channel spectral region are discussed.

PI-10. Self- and Air-Broadening, Shifts, and Line Mixing in the ν_4 and ν_2 Bands of CH_4

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A multispectrum nonlinear least squares technique¹ has been used to examine self- and air-broadening, pressure-induced shifts, and line mixing in infrared spectra of methane (CH_4) in the 6-9 μm region. The laboratory absorption spectra used in this study were recorded at high resolution (0.006-0.01 cm^{-1}) with the McMath-Pierce Fourier transform spectrometer of the National Solar Observatory. Sample temperatures ranged from 210 to 314 K, and broadening gas pressures were between 0.06 and 0.72 atm. The line broadening, shift and mixing parameters (off-diagonal relaxation matrix elements) were obtained by using the multispectrum technique to fit selected regions of 20 or more spectra simultaneously. In addition, accurate line center positions and absolute intensities were determined. The temperature dependences of the broadening and shift coefficients were determined for numerous transitions in the ν_4 and ν_2 bands of $^{12}\text{CH}_4$. Line mixing was observed in the Q branches and in the J-manifolds of the P and R branches of the ν_4 bands of $^{12}\text{CH}_4$ and $^{13}\text{CH}_4$. Line mixing parameters were also determined for 11 pairs of transitions in the weak ν_2 band of $^{12}\text{CH}_4$. The mixing parameters from the present study are compared with each other and with the results of other recent studies. This research was supported by NASA's Upper Atmosphere Research Program.

¹D. Chris Benner et al., *JQSRT* **53**, 705-721 (1995).

PI-11. Methane Spectroscopy in the Near Infrared and its Implication on Atmospheric Retrievals

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N₂-broadened half widths and pressure shifts were obtained for transitions in the Q and R branches of the 2ν₃ methane band. Laboratory measurements were done from 5985 to 6185 cm⁻¹ using spectra recorded at 0.011 cm⁻¹ resolution with a Bruker 120 HR Fourier transform spectrometer. A 140 cm gas cell was filled with methane at room temperature and N₂ as foreign gas at pressures ranging from 125 to 900 hPa. A multispectrum nonlinear constrained least squares approach based on Optimal Estimation was applied to derive the spectroscopic parameters by simultaneously fitting laboratory spectra at different ambient pressures assuming a Voigt line-shape. At room temperature, the half widths ranged between 0.030 and 0.071 cm⁻¹ atm⁻¹, and the pressure shifts varied from -0.002 to -0.025 cm⁻¹ atm⁻¹ for transitions up to J'' = 10. Especially for higher rotational levels, we find systematically narrower lines than HITRAN predicts. The new set of spectroscopic parameters is further tested with ground based direct sun FTIR measurements where fit residuals reduce by about a factor of 3-4. We report the implication of those differences on atmospheric methane measurements using high-resolution ground based FTIR measurements as well as low-resolution spectra from the SCIAMACHY instrument onboard ENVISAT. We find that for SCIAMACHY, a latitudinal and seasonally varying bias of about 1% can be introduced by erroneous broadening parameters.

PI-12. The Near Infrared (1.30 -1.70 μm) Absorption Spectrum of Methane: CW-CRDS at Room Temperature and Direct Absorption down to 77 K

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The high resolution absorption spectrum of methane has been recorded at liquid nitrogen temperature by direct absorption spectroscopy between 1.30 and 1.70 μm (5860 – 7680 cm^{-1}) using a newly developed cryogenic cell and a series of DFB diode lasers. The investigated spectral range includes part of the tetradecad and the full icosad regions for which only very partial theoretical analysis are available. The analysis of the low temperature spectrum benefit from the reduction of the rotational congestion and from the narrowing by a factor 2 of the Doppler linewidth allowing the resolution of a number of multiplets. Moreover, the energy value and rotational assignment of the angular momentum J of the lower state of a given transition have been obtained from the temperature variation of its line intensity. This procedure is illustrated in selected spectral regions by a continuous monitoring of the spectrum during the cell cool-down to 77 K, the temperature value being calculated at each instant from the measured Doppler linewidth. A short movie showing the considerable change of a spectrum during cool-down will be presented. The method applied to part of the tetradecad spectrum (5850 – 6200 cm^{-1}) has allowed an unambiguous determination of the J value of about 800 transitions.

The central part of the investigated region (1.50 and 1.60 μm) corresponds to a transparency window of particular interest for the spectral analysis of the outer planets and Titan. We have used high sensitivity CW-Cavity Ring Down Spectroscopy between 1.50 and 1.60 μm (6250 – 6680 cm^{-1}) to detect the very weak absorption transitions of methane at room temperature. The recordings were performed with a sensitivity corresponding to a noise equivalent absorption of $\alpha_{min} \sim 5 \times 10^{-10} \text{ cm}^{-1}$ and allowed for the detection of lines with an intensity smaller than $10^{-28} \text{ cm}^{-1}/(\text{molecule cm}^{-2})$ far beyond the weakest lines provided by the HITRAN database. The spectrum exhibits a highly complex and congested structure with a kind of "fractal" character and a density of transitions of a few tens per cm^{-1} . The impact of the weak newly observed transitions on the total absorption in the region is discussed. The next step will be the coupling of the cryogenic cell with the CW-CRDS technique in order to obtain the high sensitivity spectrum of methane at 77 K.

PI-13. SPECTRA, an Internet Accessible Information System for Spectroscopy of Atmospheric Gases

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We present the structure and main functional capabilities of the information system “Spectroscopy of Atmospheric Gases” (SPECTRA, <http://spectra.iao.ru>)¹. This system is developing at the Institute of Atmospheric Optics since 1999. Main goals of SPECTRA are (I) to provide an access via Internet to some spectral databases of atmospheric gases and (II) to perform some spectroscopic calculations interactively. The database of spectral line parameters of SPECTRA is based on HITRAN and GEISA databanks. In addition some original spectroscopic data for H₂O, CO₂, and H₂S are also included. Among SPECTRA options are the following:

- retrieval, extraction, and visualization of spectroscopic data;
- calculations with user defined gas mixtures;
- simulation and visualization of high and low resolution spectra;
- calculations of line positions and intensities by the effective operator method;
- download of the results to a user’s computer and/or saving these results in the system.

The system development was supported by several grants from RFBR (Russia), RFBR-PICS (Russia-France), and RFBR-NNSF (Russia-China).

¹S.N. Mikhailenko, Yu.L. Babikov, and Vl.F. Golovko, Information-calculating system Spectroscopy of Atmospheric Gases. The structure and main functions // Atmos. & Oceanic Optics, 18, 685-695 (2005)

PI-14. Some Details of the Upcoming HITRAN Updates for the New Edition of 2008

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The HITRAN2008¹ database is expected to be officially released by the end of this year. The new data will be comprised of the line lists that are already available on the web site (<http://www.cfa.harvard.edu/hitran/updates.html>) plus a number of the upcoming updates. The line-by-line lists for almost all of the 39 HITRAN molecules will be updated in comparison with the previous compilation (HITRAN2004²). The extent of the updates ranges from corrections to the representations of quantum assignments, to complete replacements or additions of parameters. In addition, two new molecules, BrO and CH₃Br, will be included. This presentation will give users an opportunity to discuss the details of the updates and to offer suggestions for future updates as well as constructive criticism.

¹The HITRAN database is supported by the NASA Earth Observing System (EOS) under the grant NAG5-13524.

²L. S. Rothman et al., JQSRT 96, 139 (2005).

PI-15. High-Resolution Spectroscopy in the Near-Infrared for Atmospheric Applications

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We present recent results of high-resolution molecular spectroscopy in the near infrared for atmospheric applications, in particular concerning reactive molecules and radicals involved in ozone chemistry (HOBr, NO₂, HO₂), water vapour H₂O and its isotopes (¹⁸O, ²D), and NH₃, using Fourier-transform and external-cavity diode-laser spectroscopy.

We will also show very recent results from broad-band cavity-enhanced spectroscopy using an incoherent broad-band source and a high-resolution Fourier-transform spectrometer.

PI-16. Spectroscopy of Carbonyl Sulfide (OCS) Near 4100 cm^{-1}

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To support planetary studies of the Venus atmosphere, we have recorded infrared absorption spectra of OCS at 0.0033 cm^{-1} resolution using a Bruker IFS 125HR Fourier transform spectrometer at the Jet Propulsion Laboratory. The spectra of normal sample OCS was acquired at ambient room temperature. Different cells were used to achieve path lengths in order to obtain optical densities sufficient to observe the weaker hot bands and isotopic bands. Line and band intensities for 29 allowed bands (12 cold bands and 17 hot bands) and two forbidden bands have been measured for five isotopologues of OCS near 4100 cm^{-1} , having 22 of them measured for the first time.

Research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contracts and cooperative agreements with the National Aeronautics and Space Administration.

SESSION III: Databases-2

III-1. JPL Millimeter and Submillimeter Spectral Line Catalog

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The spectroscopic database for the millimeter and submillimeter region has grown substantially due to continued interest in atmospheric and astrophysical remote sensing. In particular, atmospheric limb-sounding and astronomical cloud studies have raised the bar for both frequency and molecular coverage of the database. In this presentation we will outline new additions to the database with a focus on the relevant atmospheric updates. Species that are shared with the HITRAN database will be compared and contrasted with the latest version of the HITRAN compilation.

III-2. The IUPAC Water-Vapour Database

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Water is molecule number 1 in the HITRAN linelist and the correct treatment of its spectroscopic properties is crucial to the enduring success the database. Recently a task group entitled “A database of water transitions from experiment and theory” has been formed under the auspices of IUPAC to address issues related to the spectroscopy of water not just at cool, atmospheric temperatures, but also at the high temperatures required by many other terrestrial and astronomic applications.

The construction of the database has been divided into a number of tasks

1. **Energy levels and transition frequencies:** Work on this has been based on the use of the MARVEL protocol¹. The collection of data source is now well advance (see <http://chaos.chem.elte.hu/marvel/>): results for H₂¹⁸O, H₂¹⁷O and HDO are now available, those for H₂¹⁶O should be ready soon.
2. **Line intensities:** A number of comparisons have been performed and are being performed by the task group. It is my opinion, although not necessarily that of the task group, that the measurement uncertainties are such that line intensities are best obtained from *ab initio* calculations.
3. **Line profiles:** The task group is currently adopting the “Diet” protocol².
4. **Storage:** A new information system, W@DIS (see <http://saga.atmos.iao.ru/saga2/content/>), is largely constructed to store, check and manipulate the data.

Progress in this activity will be presented at the meeting.

¹T. Furtenbacher, A.G. Csaszar and J. Tennyson, *J. Molec. Spectrosc.*, **245**, 115 (2007).

²I.E. Gordon *al al*, *J. Quant. Spectrosc. Radiat. Transf.*, **108**, 389 (2007).

III-3. W@DIS: Water spectroscopy with a Distributed Information System

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Present-day processing of spectroscopic information involves the use of appropriate files for storing measured and computed data and the application of related protocols. Sometimes these files and applications are accessible via the Internet. The use of the files and the applications is not systematic, because most of them are not interrelated. To change this situation one needs to create a distributed information system (DIS) accessible via the Internet which accumulates shared knowledge and services.

The first attempt to implement such a system¹ was made at the Institute of Atmospheric Optics of the Russian Academy of Sciences in 2000. Data from HITRAN², GEISA³, and selected original sources were loaded into a relational database. Web-based interfaces were used for presentation of spectral line parameters and for calculation of spectral functions (absorption and emission coefficients, etc.). These calculations were based on well-known algorithms and the results were shared by specialists in molecular spectroscopy. The main disadvantages of this system were the absence of an explicitly specified logical structure and the absence of checking procedures during uploading of data and for the results obtained in calculations.

A significant step forward was the implementation of a distributed information system⁴ in 2005. In this system the spectroscopic tasks were roughly divided into two chains: a chain of direct and a chain of inverse problems. Both chains contain several computational tasks. The results of the first task of the inverse problem are the measurement results. At present the three active nodes of the DIS are Tomsk, St. Petersburg and Nizhnii Novgorod.

Further steps for the development of a user-friendly DIS were made during the last two years. These developments were based on the conceptual analysis of molecular spectroscopy problems. The principal aim of the domain analysis is an explicit representation of shared information components of molecular spectroscopy can be processed

¹Yu.L. Babikov *et al*, Internet collection for Molecular Spectroscopy, *Proc. of 3-rd Russian Conf. "Digital Libraries: advanced methods and technologies, digital collections"*, Petrozavodsk, 183 (2001).

²HITRAN, <http://www.cfa.harvard.edu/hitran/>

³GEISA, <http://ether.ipsl.jussieu.fr>

⁴A.D.Bykov *et al*, Distributed information system on atmospheric spectroscopy, *Geophysical Research Abstracts*, **9**, SRef-ID: 1607-7962/gra/EGU2007-A-01906, 01906 (2007).

by computers. Two types of components were considered. The first consists of spectral data such as energy levels, transition wavenumbers, intensities and certain computational data. This component is represented in the DIS in form of a relational database containing the values of the physical quantities. The second one contains the semantic data that can be processed in computers with the help of an inference engine.

A slightly simplified model was applied to the spectroscopy of water vapour and resulted in development of the information system⁵ W@DIS (<http://wadis.saga.iao.ru>). Data were collected from more than 400 information sources (articles, supplementary materials and other sources) related to water energy levels, transitions and line profile parameters. Data related to the inverse problem were uploaded and form the first type of information component. At the present time the data upload subsystem is accessible via the Internet for any interested user. The W@DIS system allows for the comparison of the stored data. Details of the related structures, as well as representation and comparison of the data will be demonstrated at the meeting.

The semantic component is formed semi-automatically during the process of data uploading. The qualitative semantic data (e.g., method of solution and related characteristics) are given by the user. The quantitative semantic data (min and max values of physical quantities, types and values of quantum numbers, and so on) are formed in W@DIS automatically. These semantic data are intended for the solution of two information tasks in molecular spectroscopy: searching the information resources and systematizing the spectroscopic resources on the basis of shared ontologies. The sense and benefit of these information tasks will also be discussed.

One of the authors acknowledges the Russian Foundation for Basic Research for financial support. This work was performed as part of the IUPAC Task Group 2004-035-1-100 "A database of water transitions from experiment and theory".

⁵A.G. Császár, A.Z. Fazliev, J. Tennyson, W@DIS - prototype information system for systematization of spectral data of water, *Abstracts of the Twentieth Colloquium on High Resolution Molecular Spectroscopy*, 270 (2007).

III-4. Updated Line-List of $^{16}\text{O}_3$ in the Range 5860 – 7000 cm^{-1} Deduced from CRDS Spectra

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The systematic study of ozone high resolution infrared spectra using CRDS technic has led to 6 recent publications ^{1, 2, 3, 4, 5, 6}. Results have been presented during the last HITRAN meeting in 2006, under the title: "CRDS spectra of ozone in the range 6000-6750 cm^{-1} ", where 5000 transitions were assigned. Since that time, many theoretical progress have been done, particularly in the predictions of band centers and rotational constants. This allows to assign more and more transitions due to weak bands. In particular, the following bands have been very recently observed and assigned: $4\nu_1+2\nu_2+\nu_3$, $4\nu_1+2\nu_2+\nu_3-\nu_2$, $5\nu_1+\nu_2+\nu_3$, $2\nu_1+3\nu_2+3\nu_3$, $4\nu_2+4\nu_3$, $3\nu_2+5\nu_3$. This corresponds now to a total of 7684 transitions (4057 energy levels). We present here these new results, with Hamiltonian and dipole moment parameters, leading to the final line-list. Examples of agreements between observed and calculated spectra are also presented.

¹S. Kassi, A. Campargue, M.-R. De Backer-Barilly and A. Barbe, *JMS*, **244**, 122-129, (2007).

²M.-R. De Backer-Barilly, A. Barbe, Vl. G. Tyuterev, D. Romanini, B. Moeskops and A. Campargue, *J. Mol. Struct.*, **780-781**, 225-233, (2006).

³A. Barbe, M.-R. De Backer-Barilly, Vl. G. Tyuterev, A. Campargue, D. Romanini and S. Kassi, *JMS*, **242**, 156-175, (2007).

⁴A. Campargue, D. Romanini, S. Kassi, A. Barbe, M.-R. De Backer-Barilly and Vl. G. Tyuterev, *JMS*, **240**, 1-13, (2006).

⁵A. Barbe, M.-R. De Backer-Barilly, S. Kassi and A. Campargue, *JMS*, **246**, 22-38, (2007).

⁶A. Campargue, A. Barbe, M.-R. De Backer-Barilly, Vl. G. Tyuterev and S. Kassi, *Phys. Chem. Chem. Phys.*, **10**, 2925-2946, (2008).

III-5. Combining HITRAN Line-By-Line, UV Cross Section and PNNL Databases for Modeling of LIBS and Raman LIDAR

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A new version of the Hitran-PC program has been developed for use in simulations of LIBS and hard target Raman LIDAR. Some of the improvements to the Hitran-PC program include the addition of PNNL IR and HITRAN cross section databases in addition to the line-by-line HITRAN database previously used. The addition of HITRAN UV cross section database made it possible to calculate the atmospheric transmission in the UV region necessary for 266 nm Raman LIDAR signal propagation simulations. The new capabilities of Hitran-PC 4.0 and main improvements to the interface will be outlined, and some results of LIBS and Raman LIDAR transmission calculations will be presented.

SESSION IV: Remote Sensing

IV-1. Implications for Molecular Spectroscopy Inferred from IASI Satellite Spectral Measurements

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IASI (Infrared Atmospheric Sounder Interferometer) is a spatially scanning Michelson interferometric emission spectrometer covering the spectrum from 645 to 2760 cm^{-1} with a resolution 0.25 cm^{-1} (Gaussian 1/e). The instrument has a demonstrated photometric accuracy of ~ 0.1 K in Brightness Temperature through much of this spectral region. We present here analyses for two IASI spectra, one acquired over the Southern Great Plains ARM site, the other over the Gulf of Mexico. Modeling of the radiance spectra with a level of accuracy consistent with that of the data provides a significant challenge. The objective here is to validate and improve the forward radiative transfer model including the associated continua and line parameters for the highly inhomogeneous radiating atmosphere. Validation of the atmospheric radiative transfer model is particularly challenging given the difficulty of providing an adequate specification of the radiating atmosphere and surface. For the present analysis radiosondes have been used for the initial guess followed by the retrieval of temperature, water vapor, methane, and carbon monoxide. The spatial and temporal variability of water vapor in the atmosphere essentially precludes the use of radiosondes for validation.

The forward model used in these analyses is LBLRTM_v11.3. The line parameters are based on HITRAN 2004 and associated updates with specific exceptions. The line parameters for carbon dioxide have been replaced by those available from Niro et al.¹ including P-Q-R line coupling. The implementation uses first order perturbation theory derived from the relaxation matrices of Niro et al. The continuum is mt_ckd.2.1. The inclusion of line coupling requires redefinition of the fundamental continuum function which will be discussed in some detail. No adjustment in the carbon dioxide line shape has yet been made for duration of collision effects. The overall results are remarkably good based on the analysis of the residuals. The need for a modification to the CO_2 line shape is clearly evident in the 2385 cm^{-1} region. The consistency between the ν_2 and ν_3 bands is remarkably good. The residuals in the 1600 cm^{-1} water vapor region are the largest in the entire spectrum presumably primarily due to issues with the spectroscopy but atmospheric inhomogeneity may play some role. Velocity broadening has not been applied in these analyses. A validation using new water vapor line strengths due to L. Coudert will be shown for comparison.

¹F. Niro, K. Jucks, J.-M. Hartmann, Spectra calculations in central and wing regions of CO_2 IR bands. IV : Software and database for the computation of atmospheric spectra: J Quant Spectrosc Radiat Transfer 95, (2005) 469-481.

IV-2. Improved Understanding of Far-Infrared Radiative Processes Using Measurements from the ARM North Slope of Alaska Climate Research Facility

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Far-infrared radiative cooling in the mid-to-upper troposphere due to water vapor contributes significantly to the dynamical processes and radiative balance that regulate Earth's climate. In the spring of 2007, the *Radiative Heating in Underexplored Bands Campaign-I* (RHUBC-I) was conducted at the Atmospheric Radiation Measurement Programs North Slope of Alaska Climate Research Facility. The experiment was designed to make detailed observations of downwelling infrared radiation in the pure rotation band of water vapor under extremely dry and cold conditions, which in many ways are similar to those found in the mid-to-upper troposphere. State-of-the-art 183 GHz microwave radiometers were also simultaneously deployed to provide the highly accurate retrievals of precipitable water vapor (PWV) that are required for the far-infrared radiative closure studies. With numerous radiosondes launched in conditions with less than 3 mm of PWV, RHUBC provided the opportunity for extensive clear-sky, high spectral-resolution comparisons between measurements and the line-by-line radiative transfer model LBLRTM. This presentation will discuss results from the RHUBC-I campaign. Specifically, we will present comparisons between LBLRTM calculations and extended-range Atmospheric Emitted Radiance Interferometer (AERI) longwave radiance observations in the far-infrared from 400 to 650 cm^{-1} . Analysis of the far-infrared spectral residuals has led to modifications to the MT-CKD water vapor foreign continuum model and adjustments to spectral line parameters relative to the current version of HITRAN. Results from the measurement-model intercomparison at 183 GHz will also be presented.

IV-3. Spectrally Resolved Measurement of the Downwelling Longwave Radiance from an High-Altitude Station: Spectroscopic Issues in the Data Analysis

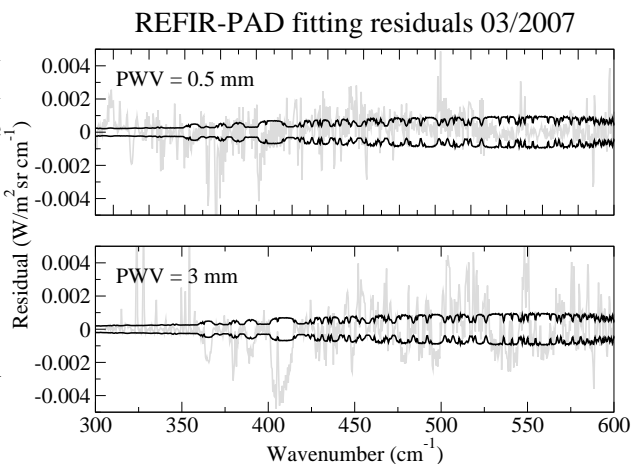
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During the ECOWAR (Earth COoling by WAter vapor Radiation) measurement campaign, held in March, 2007 from the Testa Grigia station on the italian-swiss Alps, the REFIR-PAD (Radiation Explorer in the Far-InfraRed - Prototype for Applications and Development) spectroradiometer performed spectrally resolved measurements of the downwelling atmospheric radiance in the $100 - 1100 \text{ cm}^{-1}$ spectral range, with a resolution of 0.5 cm^{-1} . Measurements were performed both in clear sky conditions and in presence of cirrus clouds, with total columnar water vapor values ranging from 0.5 to 3 mm.

The measured spectra were analyzed through a least χ^2 data fitting procedure based on the MINUIT minimization routine and the LBLRTM version 11.3 forward model, providing integrated water vapor content, cloud optical density and information on vertical water vapor and temperature profiles.

Fitting residuals from the data analysis process show significant features in the $300 - 600 \text{ cm}^{-1}$ region, that are well above measurement uncertainty, giving a hint on possible refinements both in the water vapor continuum model and spectroscopy.



IV-4. The Atmospheric Chemistry Experiment, ACE: Latest Results

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The Canadian ACE (Atmospheric Chemistry Experiment) mission has a high resolution (0.02 cm^{-1}) Fourier transform spectrometer (FTS) in low earth orbit. ACE was launched by NASA in August 2003 and the FTS continues to operate without any degradation in performance. The primary ACE mission goal is the study ozone chemistry in the stratosphere although it is making a wide range of other measurements, for example, of organic molecules in the troposphere. Some of the recent results from ACE will be presented, emphasizing the use of HITRAN data for retrievals. ACE has now measured about 18000 occultations and we have co-added 224782 pure solar spectra to produce the ACE solar atlas in the $750 - 4400\text{ cm}^{-1}$ spectral region.

IV-5. Spectroscopic Issues for the Atmospheric Chemistry Experiment (ACE)

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The Atmospheric Chemistry Experiment (ACE), otherwise known as SCISAT-1, is a Canadian-led satellite mission for remote sensing of the Earth's atmosphere. The satellite was launched August 12, 2003, and science operations began in February 2004. The primary instrument on board is a high-resolution (0.02 cm^{-1}) Fourier transform spectrometer (ACE-FTS) operating in the infrared ($750\text{--}4400\text{ cm}^{-1}$). The measurement technique employed is solar occultation. In preparation for the next processing version (version 3.0) of the ACE-FTS retrievals, the spectroscopic data for some key molecules have been evaluated. For CO_2 , there appears to be a 1-2 % variability in the intensities of lines used for pressure/temperature retrievals from the ACE-FTS. Very weak lines of H_2O , used in the retrieval of water below about 12 km, exhibit extremely bad internal consistency in their intensities. New spectroscopic parameters for some of these weak water lines have been generated from the ACE-FTS spectra. HNO_3 spectroscopic data in different wavenumber regions are not internally consistent. A scaling factor of 8.5 % is applied to the intensities of nitric acid lines near 1700 cm^{-1} in order to achieve consistency with the HNO_3 lines near 900 cm^{-1} . The spectroscopic data for C_2H_6 is incomplete in HITRAN 2004 (including the C_2H_6 update). In particular, spectral features for ethane near 2967 cm^{-1} are missing in HITRAN, which causes problems in the retrievals for CH_3Cl . Weak CH_4 lines in the ACE-FTS spectra exhibit line shape problems that may be a consequence of line mixing. Bad residuals from these methane lines complicate the retrievals for a number of weak absorbers.

IV-6. Applying Spectroscopy to Global Change: Isotopic Ratio Measurements of Ambient Carbon Dioxide and Methane

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Real time methods to monitor the stable isotopic ratios of carbon dioxide and methane are needed to quantify the sources and sinks of these important greenhouse gases. High resolution molecular spectroscopy provides an attractive solution. However, this is an extreme instrumental challenge since the ratios need to be measured with an accuracy of approximately one part in ten thousand or 0.1%. We use tunable infrared laser differential absorption spectroscopy with quantum cascade (QC) lasers to address this challenge. QC lasers are attractive optical sources since they do not need cryogenic fluids, they have stable single mode spectral output and offer optical simplicity.

We have used a pulsed-QCL instrument to perform long term (>10 months) monitoring of ambient air from the roof top of our laboratory with time resolution of one second. The resulting data set shows both short term and long term isotopic variations. We observe clear seasonal changes in both $^{13}\text{C}/^{12}\text{C}$ and $^{18}\text{O}/^{16}\text{O}$. We have recently extended this technique to the even more challenging case of $^{13}\text{CH}_4$ using continuous wave QCLs. Preliminary results of these measurements will be presented as well.

Poster Session II

PII-1. Detection of NO₂ Using an External Cavity, Tunable, CW Quantum Cascade Laser Employing Wavelength Modulation Spectroscopy Techniques

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An external cavity, tunable, CW Quantum Cascade Laser operating at room temperature was tested employing wavelength modulation spectroscopy techniques. The goal is to employ this laser to detect environmental NO₂ with high sensitivity and selectivity. The laser operates in the region 1625 cm⁻¹ to 1645 cm⁻¹. We report the first to seventh harmonic detection of the 1642 cm⁻¹ line of water. The water lines are identified and modeled after the HITRAN database. The data on water, preliminary NO₂ data, and the performance of the laser for trace gas detection will be presented.

PII-2. Evolution of OH Spectroscopic Parameters in Theory and in Practice

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While being a simple diatomic molecule, the hydroxyl radical hardly exhibits simple spectra. In this presentation, the issues concerning the infrared emission lines (Meinel system) of the OH molecule will be discussed. These emission lines are an invaluable tool in many applications including the study of non-LTE upper atmosphere emissions, atmospheric gravity waves, stellar oxygen abundance, planetary atmospheres, etc. While the spectroscopic parameters of the Meinel system have been studied for many decades, the physics behind the spectrum had become hidden behind the equations in some of the recent publications. That eventually led to a gap in the treatment of the OH bands by spectroscopists and atmospheric scientists. This presentation will be aimed at closing that gap. In particular, the unusual behavior of the dipole-moment function due to the strong vibration-rotation interaction will be critically reviewed. The status of the current OH line list in the HITRAN database will be discussed and future improvements and their sources will be presented.

PII-3. N₂-Broadening of ν_5 Band Transitions of HNO₃ in the Region from 841 to 931 cm⁻¹

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A number of satellite instruments are measuring nitric acid, HNO₃, in the Earth's atmosphere. In order to do retrievals of temperature and concentration profiles, the spectral parameters for many thousands of HNO₃ transitions must be known. Currently on the HITRAN database the air-broadened half-width is defaulted to 0.11 cm⁻¹ atm⁻¹. To help ameliorate this situation, complex Robert-Bonamy calculations were made to determine N₂-broadened half-widths and their temperature dependence for some 5000 transitions of HNO₃ in the ν_5 band. The intermolecular potential is a sum of electrostatic terms (dipole-quadrupole and quadrupole-quadrupole), and the atom-atom potential expanded to eighth order. The trajectory parameters were adjusted to yield better agreement with measurement. Velocity integrated calculations were made at seven temperatures (200, 225, 275, 296, 300, 375, 500 K) in order to determine the temperature dependence of the half-widths. The data are compared with measurements of Goyette et al. (J. Quant. Spectrosc. Radiat. Transfer 60, 77, 1998). The average percent difference between the measured and calculated half-widths is -0.31. The temperature, and rotational state dependence of the half-width are investigated.

PII-4. Retrieval of H¹⁵NO₃ Vertical Atmospheric Distribution from MIPAS/ENVISAT Limb-Emission Measurements

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Because of atmospheric interest, the HNO₃ molecule has been the subject of a number of spectroscopic studies, particularly in the 11.2 μm spectral region which is widely used for atmospheric retrievals of ¹⁴N nitric acid. However, accurate spectral line parameters have only recently been generated for the isotopic species H¹⁵NO₃. Thanks to these parameters, the Q-branch of the ν₅ band of H¹⁵NO₃ was identified (near 871 cm⁻¹) in high signal-to-noise ratio atmospheric limb-emission spectra measured by the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on-board the European environmental research satellite ENVISAT. We have thus exploited this ν₅ Q-branch to retrieve from MIPAS spectra the atmospheric vertical distribution of the H¹⁵NO₃ isotopologue. Due to the very low intensity of the spectral feature used for retrieval, it was necessary to develop an ad-hoc inversion algorithm for the H¹⁵NO₃ profile retrieval. This algorithm, based on a regularized sequential Kalman filter, permitted retrieval of profiles of the ¹⁵N/¹⁴N isotopic ratio, averaged over different latitudinal bands and time intervals, for the altitude range 18 - 42 km. The first retrieval attempts show a reasonable accuracy (about 10% from 20 to 25 km) and a clear depletion of H¹⁵NO₃ above 25 km altitude.

PII-5. HNO₃ Spectroscopic Parameters in the 600 - 950 cm⁻¹ and 1300 - 1360 cm⁻¹ Spectral Regions

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In an earlier study¹ the parameters available for HNO₃ in the HITRAN spectroscopic database have recently been revisited in the spectral range corresponding to the MIPAS spectral range. These updates involve the line positions for the ν_5 and $2\nu_9$ bands, and the overall intensities for the 830 - 1800 cm⁻¹ region. However, when examining in details comparisons between the observed spectra recorded by MIPAS and the calculated ones, some disagreements in the MIPAS residual can be still observed. The goal of the present talk is to solve these problems. For the 600-950 cm⁻¹ spectral region, a new HNO₃ database was generated by analyzing spectra of nitric acid broadened by N₂ recorded using the Bruker FTIR spectrometer of the LISA laboratory. From the results of this first study, two hot bands ($\nu_5+\nu_7-\nu_7$ and $\nu_5+\nu_6-\nu_6$) are now included in the new database. The intensities were updated for the ν_6 and ν_8 bands at 646.8 and 763.1 cm⁻¹ respectively. Accurate line broadening parameters were implemented using a new calculation². Finally, it was possible to identify, for the first time, and model correctly line mixing effects in the Q branch region of the $\nu_5+\nu_9-\nu_9$ hot band (at 885.4 cm⁻¹).

For the 1260 - 1350 cm⁻¹ region, the goal of this work was to get better line positions and intensities for the ν_3 and ν_4 interacting cold bands located at 1303.071 and 1326.182 cm⁻¹ respectively as compared to those achieved few years ago³. The theoretical model accounts for the vibration-resonances which link the energy levels of the 4¹ and 3¹ bright vibrational states together with those of several dark interacting states. Very preliminary results will be presented.

¹Flaud JM, Brizzi G, Carlotti M, Perrin A, Ridolfi M. Atmos. Chem. Phys. 2006; 6: 1-12

²R.R. Gamache and A. Laraia: poster presentation

³A.Perrin, O.Lado-Bordowski and A.Valentin, Mol. Phys. 67, 249 (1989)

PII-6. First List of Line Positions and Intensities for the ν_3 Band of Trans-Formic Acid Near 5.6 micrometer

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The 5.6 μm spectral range can now be used to detect simultaneously formic acid (HCOOH) and formaldehyde (H₂CO) in the troposphere using quantum cascade laser techniques.¹ However, no reference spectroscopic information is currently available for these species at 5.6 μm in databases such as HITRAN.² The goal of the present study is to fill this gap for the ν_3 band of formic acid centered at 1776.833 cm^{-1} , following our recent contributions for HCOOH in the 9 μm region.³ Using high resolution Fourier transform spectra of formic acid recorded in Brussels and relying on the results of a previous study,⁴ we performed an extended analysis of the ν_3 band of trans-HCOOH. Absolute line intensities were also obtained, taking the contribution of the dimer (HCOOH)₂ into account.^c The ν_3 band is significantly perturbed by several dark states. The theoretical model that we used to compute the line positions and intensities reproduced most of the observed perturbations. A list of individual line positions and intensities was generated, which we hope will be useful for atmospheric applications.

¹S.C. Herndon, M.S. Zahniser, D.D. Helson, J. Shorter, J.B. McManus, R. Jimenez, C. Warneke, and J.A. de Gouw, *J. Geophys. Res.* D112 (2007) D10S03

²L.S. Rothman *et al.*, *J. Quant. Spectrosc. Radiat. Transfer* 96 (2005) 139-204

³J. Vander Auwera, K. Didriche, A. Perrin, and F. Keller, *J. Chem. Phys.* 126 (2007) 124311; A. Perrin, J. Vander Auwera, *J. Quant. Spectrosc. Radiat. Transfer* 108 (2007) 363-370

⁴W.H. Weber, P.D. Maker, J.W.C. Johns, and E. Weinberger, *J. Mol. Spectrosc.* 121 (1987) 243-260.

PII-7. Line Positions and Intensities in the ν_{12} Band of Ethylene Near 1450 cm^{-1} : an Experimental and Theoretical Study

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Recently, we built a tensorial formalism^{1,2} adapted to the spectroscopy of X_2Y_4 molecules. It is based on formalisms developed in Dijon for spherical-top molecules³. This approach has the advantages to allow a systematic development of rovibrational interactions and to make global analyses easier to perform. We used this tool to carry out an analysis of the ν_{12} band of $^{12}\text{C}_2\text{H}_4$ near 1450 cm^{-1} , both in frequencies and intensities. 1240 line positions and 871 intensities, measured in a set of spectra recorded in Brussels, were fitted with global root mean square deviations of $1.6 \times 10^{-4}\text{ cm}^{-1}$ and 1.88 %, respectively

¹W. Raballand, M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.* 217 (2003) 239-248.

²Ch. Wenger, W. Raballand, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer* 95 (2005) 521-538.

³V. Boudon, J.-P. Champion, T. Gabard, M. Loëte, F. Michelot, G. Pierre, M. Rotger, Ch. Wenger and M. Rey, *J. Mol. Spectrosc.* 228 (2004) 620-634.

PII-8. $^{14}\text{CO}_2$ Laser Heterodyne Measurements of Frequencies and Intensities of Ethane at $12\mu\text{m}$

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The absolute infrared intensities of transitions in the ν_9 band of ethane have long been a subject of controversy (Gunson 1996, Daunt 1984, Henry 1983, Auwera 2007, and references therein). Improving the ethane $12\mu\text{m}$ database is one of the goals of this work. The spectra here acquired was obtained using the NASA Heterodyne Instrument for Planetary Wind And Composition (HIPWAC) in a laboratory setting. HIPWAC, in this environment, makes use of a blackbody source and a gas absorption cell. Observations were carried out from P(10) at $858.1583905\text{ cm}^{-1}$ to P(32) at $839.1958112\text{ cm}^{-1}$ of the 646 laser. The observational range is $\pm 3\text{GHz}$ centered on each laser line.

HIPWAC has the ability to measure spectra by using infrared heterodyne techniques, in which an infrared source is combined with a laser local oscillator and focused on a photomixer, where the difference frequency between the source and laser is retrieved and analyzed. Using these techniques HIPWAC is able to achieve a very high resolution ($\lambda/\Delta\lambda > 10^6$) and a high frequency specificity ($> 10^{-8}$) in order to study low-pressure gases. The spectra was retrieved using an Acoustic-Optical Spectrometer (AOS) with a sampling interval of 1 MHz. The detector was a liquid Helium cooled HgCdTe Photomixer. The ethane was research grade (99.96 %) obtained from Matheson Gas Products. The gas was contained in a 30 cm straight-path cell with ZnSe windows. The gas pressure was 0.709 Torr, as measured by an MKS Baratron gauge, at a temperature of 26 degrees Celcius. Additional measurements were also done at 1.4 Torr and 2.8 Torr. The spectra acquired is double sided and was fitted using an IDL program. The quantum assignments were taken from previous atlases (Tennessee/GSFC and GEISA).

Currently, similar measurements are also being done on Allene and OCS. In the future we would like to incorporate Quantum Cascade Lasers in our system to replace our CO_2 gas lasers. Quantum Cascade lasers are very small solid-state devices with an output power of about 100 mW and limited tunability.

PII-9. Line Intensities of Methanol in the 400 cm^{-1} Region

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High-resolution infrared absorption spectra of methanol (CH_3OH) has been recorded between $400 - 700\text{ cm}^{-1}$, with the Bruker IFS 125 HR Fourier transform spectrometer, located at the Jet Propulsion Laboratory, using a 20.26 cm glass cell with wedged, high-density polyethylene windows. Line intensities in the 400 cm^{-1} region, retrieved using a non-linear least square line fitting program, will be presented.

Research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contracts and cooperative agreements with the National Aeronautics and Space Administration.

PII-10. The Acetylene Laboratory IR Spectrum: Quantitative Studies and Databases

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The acetylene molecule C_2H_2 shows numerous vibration-rotation bands throughout the IR spectrum. Vibrational levels of C_2H_2 are grouped into clusters almost regularly spaced every 700 cm^{-1} , from the fundamental ν_5 band, at $13.6\ \mu\text{m}$, up to the visible. Several IR spectral regions where C_2H_2 bands occur have been extensively studied in the past years, mainly in order to obtain absolute individual line intensities and to improve spectroscopic databases as HITRAN or GEISA. This quantitative spectroscopy work is performed with the aid of Fourier transform interferometers to obtain absorption spectra, and using a multispectrum fitting procedure to retrieve line parameters from these spectra. For usual applications, a semi-empirical model based on the Herman-Wallis factor is used to generate line lists dedicated to spectroscopic databases. This poster gives a summary of all the spectral regions studied for acetylene $^{12}C_2H_2$, pointing out the current state of the spectroscopic databases HITRAN/GEISA, and the recent works done through the collaboration between the LPMAA (Paris), the GSMA (Reims), the LADIR (Paris) and the LTS (Tomsk).

Works in progress and projects will also be presented. Data available in the literature, or obtained in the recent works, have been compiled to set up line lists usable for applications and dedicated to databases.

PII-11. Methyl Bromide $^{12}\text{CH}_3^{79}\text{Br}$ and $^{12}\text{CH}_3^{81}\text{Br}$ around 10- μm : a Complete Set of Parameters for Atmospheric Detection

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Methyl Bromide (CH_3Br) has the highest tropospheric concentration among all long-lived organobromides, making it the primary source of bromine to the stratosphere. Bromine radical in the stratosphere has been shown to contribute significantly to stratospheric ozone loss through coupled reactions with ClO , HO_2 and NO_2 radicals. Methyl bromide is a trace gas that could be detected and quantified in atmospheric spectra. Line positions, intensities, self- and N_2 -broadening coefficients from a recent work ¹ in the 10- μm spectral region have been added in the HITRAN and GEISA databases for around 15000 transitions. A work based from these data is still in progress to detect CH_3Br for example in ACE spectra.

This poster summarizes several works in the 10- μm spectral region using high resolution Fourier Transform spectra recorded at LADIR (Paris). Studies on line positions, self- and N_2 -broadening coefficients, line intensities, line mixing at room temperature ², and temperature dependence exponents of the self- and N_2 -broadening coefficients ³, and finally line mixing at lower temperature (180-300 K)⁴ will be presented.

¹D. Jacquemart, F. Kwabia Tchana, N. Lacome, I. Kleiner. A complete set of line parameters for methyl bromide in the 10- μm region. JQSRT 2007;105:264-302.

²H. Tran H, D. Jacquemart, J.-Y. Mandin, N Lacome. Line-mixing in the ν_6 Q branches of methyl bromide self- and nitrogen-broadened: experiment and modelling. JQSRT 2008;109,119-131.

³D. Jacquemart, H. Tran. Temperature dependence of self- and N_2 - broadening coefficients of CH_3Br . JQSRT 2008;109:569-579.

⁴L. Gomez Martin, H. Tran, D. Jacquemart. Line-mixing in the ν_6 Q branches of methyl bromide nitrogen-broadened at low temperature: experiment and modelling. JQSRT (under redaction).

PII-12. Extracting Accurate Molecular Spectroscopic Parameters From High Resolution IR Laboratory Spectroscopy.

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We report on our molecular spectroscopy effort to determine frequencies, intensities, shapes and broadening in fundamental and low-lying hot band transitions for molecules of interest to contemporary planetary atmospheric investigations. The laboratory measurements, obtained with the NASA/GSFC Heterodyne Instrument for Planetary Wind and Composition (HIPWAC), are described in a companion paper in this session (see Blass et al.) which also compares our results to those of other researchers (e.g., Vander Auwera et al.). Herein we present the analysis methodology and interpretation of the laboratory measurements.

We identified molecular species of significance to current outer-planet missions such as the Cassini Mission to Jupiter, Saturn and Titan: ethane (C_2H_6), including both normal and primary hot band (i.e., ν_9 and $\nu_9 + \nu_4 - \nu_4$); ethylene (C_2H_4); and allene (C_3H_4). The laboratory measurements which are the basis for the results reported herein were obtained at a spectral resolution of 0.00003 cm^{-1} ($\sim 1\text{MHz}$) at $12\text{ }\mu\text{m}$. At this spectral resolution, the rotation-vibration transitions measured under laboratory conditions (ambient temperature and ~ 1 Torr pressure) are fully resolved and identified without ambiguity. The principal objective is to provide critical laboratory truth for the interpretation of infrared spectral observations of the Cassini mission, follow on missions to Titan and the outer planets, and in the re-interpretation of mid-IR emission spectra from Voyager IRIS, ISO, and ground based IR data of the outer planets. Resultant line intensities ($<3\%$ accuracy) and line frequencies ($<0.0001\text{ cm}^{-1}$ accuracy) will improve existing line atlases (e.g., Univ. of Tennessee, HITRAN). We discuss the analysis methodology and interpretation of the HIPWAC laboratory measurements, establish the statistical errors in the extraction of the spectroscopic parameters, and demonstrate the impact on modeling high-resolution infrared spectra of outer planet atmospheres such as Titan. We gratefully acknowledge the support of the NASA/Planetary Atmospheres Program.

PII-13. Calculation of Refraction Indices of Planetary Atmospheres Using HITRAN

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Calculations of the refractive indices from the visible to far-infrared for Earth and other planetary atmospheres are presented. The calculations have been performed using a recently developed fortran code that computes the real part of the refractive indices using as input the oscillator strengths (location on a wavenumber (wavelength) axis plus the strengths related to Einstein coefficients, transition moments, etc) from the HITRAN database. The absorption spectrum is the imaginary part of the refractive index, which essentially is a Kramers-Kronig transform of the real part. These are plugged into the numerator and denominator of the standard oscillator formula, corrected for the Claussius-Mossotti terms. The formulation used in this work is based on the work by Mathar¹ and developed in support of astronomical observations.

In this paper the effect of the variation of the refraction indices with wavelength and atmospheric conditions and comparisons with a previously developed model by Collavita et al.² will be be discussed.

¹R. Mathar *Applied Optics* **43**(4), 928-932, 2004.

²Collavita et al. *Publications of the Astronomical Society of the Pacific* **116**, 876-885, 2004.

PII-14. Examine Climate Models by Using Infrared Spectrum

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We examine global climate models by comparing the satellite-observed high resolution global infrared spectra with the model-simulated counterpart. Because the top-of-the-atmosphere outgoing Earth thermal emission at different frequencies is sensitive to different geophysical variables (temperature, water vapor and other greenhouse gas concentrations, clouds, etc.) at various levels, a comparison of observed and simulated spectra is as challenging as examining a variety of model-simulated geophysical variables simultaneously. Thus, the ability of climate models to replicate the observed spectra provides a strict metric for model validation. This approach adopts a forward radiative transfer calculation and thus avoids the uncertainties associated with retrieving geophysical variables from the radiance measurement.

After ensuring consistency in the sampling of the observed and simulated spectra and a proper representation of cloud vertical distribution, the infrared spectra simulated from a state-of-the-art Geophysical Fluid Dynamics Lab climate model are shown to yield a good agreement with those measured by the Atmospheric Infrared Sounder onboard Aqua satellite, in terms of global and regional means. The radiance discrepancies in the water vapor and carbon dioxide ν_2 bands are consistent with the model biases in atmospheric water vapor and temperature. Furthermore, an examination of the seasonal covariations of the infrared spectra and surface temperatures demonstrates the need and a method to use spectrally resolved radiance to understand and constrain model sensitivity. This study shows that infrared spectrum forms an advantageous means for climate model validation. The study also provides an example of the climatic applications using spectroscopic observations and the molecular absorption database.

PII-15. Initial Results from SOFIE/AIM

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SOFIE (the Solar Occultation For Ice Experiment) has been operating since May 2007 onboard AIM (the Aeronomy of Ice in the Mesosphere satellite). SOFIE measurements target the polar mesosphere, where noctilucent clouds form each summer. Increases in the frequency and brightness of these ultra-high clouds have been attributed to global climate change, but conclusive evidence is lacking, and relatively little is known about the processes governing their formation. SOFIE is now providing key measurements to advance our understanding of these clouds and their environment. The instrument acquires limb path transmittances in 16 spectral bandpasses from the UV to the IR. Vertical profiles of cloud properties, temperature, water vapor, ozone, methane and nitric oxide are inverted from these transmittance measurements. With over a year of observations in hand, we now have information leading to a better understanding of the formation of noctilucent clouds, including the first ever measurements of the cosmic dust layer. In this presentation we describe the instrument, outline the retrieval process, and discuss preliminary science results from the SOFIE experiment.

PII-16. Surface Pressure Measurements Using Differential Absorption LIDAR with Broad Laser Lines

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The monochromatic peak of an isolated absorption line in the earth's atmosphere is insensitive to pressure changes with a constant path length or altitude. The most sensitive positions to measure surface pressure change are on the sideline and the troughs. Conversely, the monochromatic peak of an isolated absorption line is sensitive to pressure changes at the same pressure altitude. Keeping the measurements at the same pressure altitude is the nature of remote sensing of surface pressure from a space platform. The thickness of the earth's atmosphere is larger at a high-pressure area than a low-pressure area from a space platform. This implies as the surface pressure changes so does the total path length. This study examines the variable of pressure in Beer-Lambert law to observe its influence in an exponentially ascending pressure gradient from airplane altitudes to space platforms. While using Differential Absorption Lidar (DIAL), it takes the approach of calibration using ground station pressure and then characterizing the change of the absorption line due to changes in pressure. In both cases, same pressure altitude or same path length, it is advantageous to use wide laser lines to minimize errors and to target pressure information.

SESSION V: Laboratory Spectroscopy

V-1. Quantitative Measurement of Integrated Band Intensities Of Benzene (C₆H₆) Vapor in the Mid-Infrared at 278, 298 and 323 K

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Pressure broadened (1 atm. N₂) laboratory spectra of benzene vapor (in natural abundance) were recorded at 278, 298, and 323 K, covering 600-6500 cm⁻¹. The spectra were recorded at a resolution of 0.112 cm⁻¹ using a commercial Fourier transform spectrometer (FTS). Pressure of each benzene vapor sample was measured using high precision capacitance manometers and a minimum of nine sample pressures were recorded for each temperature. The samples were introduced into a temperature-stabilized static cell (19.94(1) cm pathlength) hard-mounted in the spectrometer. From these data a fit composite spectrum was calculated for each temperature. The number density for the three composite spectra was normalized to 296 K. The spectra give the absorption coefficient (cm² molecule⁻¹, naperian units) as a function of wavenumber. Integrated band intensities (cm molecule⁻¹ and atm⁻¹ cm⁻²) for intervals corresponding to the stronger benzene bands were derived and are compared with previously reported values. We discuss and quantify error sources and estimate our systematic errors to be 3% for stronger bands. The measured absorption coefficients and integrated band intensities are useful for remote sensing applications such as its measurement in planetary atmospheres and assessment of the environmental impact of terrestrial oil fire emissions, and studies of dense parts of envelopes surrounding interstellar molecular clouds. We focus on the ν_4 band (Herzberg notation) at 674 cm⁻¹, the strongest infrared band that is currently being measured in Titan's stratosphere by the Composite InfraRed Spectrometer (CIRS) during Cassini spacecraft fly-bys, and we compare our results with previously reported measurements. The intensity (cm⁻²atm⁻¹) for the ν_4 band integrated from 615 to 735 cm⁻¹ is 427±13 at 278 K, 428±13 at 287 K, and 426±13 at 323 K, indicating no dependence with temperature. However, Q branch absorption coefficients (the feature measured by CIRS) are 1.3 higher at 278 K than at 323 K.

V-2. Pressure-Broadening of Water Lines in the THz Frequency Region: Improvements and Confirmations for Spectroscopic Databases

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The interaction between the electromagnetic radiation and the molecular species present in the earth atmosphere is of fundamental importance for studying the composition of the atmosphere itself and its evolution. Among all the constituents of the terrestrial atmosphere, water, even if it is a minor component, plays a significant role in the absorption of radiation and it is involved in many atmospheric phenomena by affecting atmospheric warming and cooling, weather and climate, electromagnetic waves propagation.

Remote sensing applications require the spectroscopic parameters of the various atmospheric constituents to be known accurately. These parameters are collected in spectral databases such as HITRAN and, among them, the collisional broadening parameters have a crucial influence on reduction of remote sensing data. Actually, the largest sources of uncertainty in retrieved profiles are the pressure-broadening coefficient itself and its temperature dependence. HITRAN values are taken from measurements, when they are available, but in most cases come from calculations. Air broadening and shift, are deduced from a semiclassical treatment of the H₂O collisions with N₂ or O₂, while self broadening parameter is obtained by an average of the J dependence of the existing experimental data.

In order to check the accuracy of the existing values, measurements of pressure-broadened half-widths have been carried out in the THz frequency region. More precisely, the following transitions have been investigated: $J = 3_{1,2} \leftarrow 3_{0,3}$ (1.097 THz), $1_{1,1} \leftarrow 0_{0,0}$ (1.113 THz), $7_{2,5} \leftarrow 8_{1,8}$ (1.147 THz), $3_{1,2} \leftarrow 2_{2,1}$ (1.153 THz), $6_{3,4} \leftarrow 5_{4,1}$ (1.158 THz), $3_{2,1} \leftarrow 3_{1,2}$ (1.163 THz), $8_{5,4} \leftarrow 7_{6,1}$ (1.168 THz), $7_{4,4} \leftarrow 6_{5,1}$ (1.173 THz), $8_{5,3} \leftarrow 7_{6,2}$ (1.191 THz), and $6_{3,3} \leftarrow 5_{4,2}$ (1.542 THz). Since we focus on application to the Earth's atmosphere, nitrogen, oxygen and water have been considered as perturbing gas. Measurements were found in good agreement with semiclassical calculations.

Our results show that old measurements are sometimes not very accurate and that the HITRAN self broadening parameters obtained by assuming a J dependence can involve large errors. Indeed, simple semiclassical calculations performed for more than 1500 rotational water lines with frequency lower than 1000 cm⁻¹ cast doubts on many

self broadening values reported in the HITRAN database, while are in good agreement with experiment. On the whole, we can conclude that when no reliable measurement is available semiclassical calculations should be resorted to also for the self broadening parameter.

V-3. From Matrix Isolation Spectroscopy to First Observation of the CO₂ 628 Isotopologue ($\nu_2 + \nu_3$) Band in the Atmosphere Of Venus

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Due to its interest for atmospheric studies, carbon dioxide is probably the molecule whose IR spectrum has been the most extensively studied. However, recent observation and identification of a new absorption band, at 3.35 μm , detected by SOIR on board ESA Venus Express mission was not straight forward. It was finally attributed to the 628 isotopologue of carbon dioxide, as the result of a collaboration between different teams involving different techniques^{1, 2, 3, 4}. One of these, matrix isolation spectroscopy, coupled to gas phase spectroscopic methods, provides a useful and easy way to help identifying spectral features of individual absorbers from dense spectra. The process requires evaluation of the matrix effect environment on the electric potential driving the nuclear motions, calculation of the ro-vibrational energies and finally determination of the selection rules from group theory, for allowed transitions. Comparison of observed and calculated transitions from Laser Induced fluorescence validated this method for carbon dioxide and ozone⁵. More elaborate methods can then be used to determine the line parameters such as intensity and widths from observed spectra to fully characterize the observed absorptions⁶. Taking into account those newly observed transitions may help refining the modeling of green house effect on Venus and on Mars, it could improve

¹J. L. Bertaux, A. C. Vandaele, V. Wilquet, F. Montmessin, R. Dahoo, E. Villard, O. Korablev and O. Fedorova *Icarus* **195**(28-33), 2008.

²V. Wilquet, A. Mahieux, A. C. Vandaele, V. Perevalov, S. Tashkun, A. Fedorova, F. Montmessin, R. Dahoo and J. L. Bertaux *J. Q. S. R. T.* **109**(895-905), 2008.

³G. L. Villanueva, M. J. Mumma, R. E. Novak and T. Hewagama *Icarus* **195**(34-44), 2008.

⁴G. L. Villanueva, M. J. Mumma, R. E. Novak and T. Hewagama *J. Q. S. R. T.* **109**(833-894), 2008.

⁵P. R. Dahoo, H. Chabbi, A. Lakhlifi and J. M. Coanga *J. Mol. Struct.* **786**(157-167), 2006.

⁶R. A. Toth, C. E. Miller, L. R. Brown, V. Malathy Devi and D. Chris Benner *J. Mol. Spec.* **243**(43-61), 2007.

the retrieval of methane, whose main absorption features overlap with the 628 CO₂ lines. The presentation will focus on the methods described above applied to the retrieval of the line parameters, positions and intensities of the observed rovibrational transitions from spectra recorded by SOIR in the atmosphere of Venus above 70 km. We will briefly describe the instrument and recall the SOIR technique. Then we will focus on the retrieval of the line positions from matrix isolation spectroscopy and analysis of symmetry to determine the allowed selection rules. Finally, results of calculations of the line parameters and the Hermann-Wallis factors for the observed band will be presented with a glance at results obtained for other isotopologues detected on Mars from earth observations ⁷.

⁷G. L. Villanueva, M. J. Mumma, R. E. Novak and T. Hewagama *J. Q. S. R. T.* **109**(833-894), 2008.

V-4. Methane for Atmospheric and Planetary Applications: What Spectroscopic Parameters Do We Need?

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The spectroscopic knowledge of methane is important to study the greenhouse effect and some planetary atmospheres. The analysis of atmospheric and planetary spectra can be performed through line-by-line computations or through cross-sections data. When available with enough accuracy, line parameters allow calculations under any conditions of pressure, temperature and absorption path. Many works have been published on methane, leading to a huge line list (more than 250,000 transitions) in the HITRAN 2004 database. However, for most of the transitions between 1 and 1.65 μm , energies of the lower levels (E'') are unknown. Consequently, line intensities known at the standard temperature (296K) cannot be calculated for the temperatures of planetary atmospheres or of high layers of our atmosphere. On the other hand, cross sections can be used with enough accuracy only when the experimental conditions are close enough to those of the studied atmosphere. This requires a set of cross sections for each experiment and atmospheric conditions.

As example, new measurements of methane cross sections had to be recently performed¹ under Titan surface similar conditions and matching the experimental recording conditions of the DISR (DISR-Descent Imager/Spectral Radiometer) of the Huygens probe landed in January 2005 on Titan. The experimental device used to record these cross sections is presented, together with some typical results and their use to deduce methane amount on Titan surface.

To get more versatile data, we propose a method to deduce E'' values from absorption spectra, without knowing complete assignments, but precise enough to allow calculation of line intensities at any temperatures of interest. To test the feasibility of this method, two spectra (at 120K and 300K) are simultaneously adjusted using a multispectrum fitting procedure in which E'' is a free parameter. Some examples of E'' retrievals for lines already assigned in HITRAN show the efficiency of the method.

¹D. Jacquemart, E. Lellouch, B. Bzard, C. De Bergh, A. Coustenis, N. Lacome, B. Schmitt, and M. Tomasko. New laboratory measurements of CH_4 in Titan's conditions and a reanalysis of the DISR near-surface spectra at Huygens landing site. *Planetary and Space Science Special issue 2 on Titan as seen by Huygens 54/5,613-623 (2008)*.

V-5. The High Resolution Infrared Spectrum of $^{34}\text{SO}_2$ up to 4000 cm^{-1}

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The infrared spectrum of sulfur dioxide is of interest both for the earth (volcanic eruptions in particular) and planetary (Venus, Io) atmospheres. While the spectrum of the normal species, $^{32}\text{SO}_2$, has been very well studied and an excellent set of molecular constants obtained, this is not the case for the rarer isotopic species, $^{34}\text{SO}_2$, the abundance of which is about 4.2% of the normal species.

In order to improve our knowledge of the $^{34}\text{SO}_2$ spectrum we have studied a sample of SO_2 enriched to 95% in ^{34}S at high resolution (0.0019 cm^{-1}) over a wavenumber region including all the fundamental bands, the relatively strong combination bands $\nu_2+\nu_3$ and $\nu_1+\nu_3$ as well as the weaker $2\nu_3$ and $2\nu_1+\nu_3$ bands. Also the hot bands $2\nu_2-\nu_2$, $3\nu_2-2\nu_2$, $\nu_1+\nu_2-\nu_2$, $\nu_2+\nu_3-\nu_2$, $\nu_1+\nu_2+\nu_3-\nu_2$ were analysed. In this way, an accurate set of assigned lines was derived. The experimental energy levels were fitted leading to an accurate set of rotational constants for the (000), (010), (020), (030), (100), (001), (101), (201) vibrational states. From these constants, equilibrium rotational constants were derived and an accurate equilibrium structure determined. Finally, line intensities are being measured and preliminary results concerning this last point will be presented.

V-6. Absolute Line Intensities and Accurate Line Broadening Parameters for the 5.7 μm and 3.6 μm Bands of Formaldehyde

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The goal of this study was to achieve absolute line intensities and reliable line broadening parameters for the strong 5.7 μm and 3.6 μm bands of formaldehyde (H_2CO) and to generate, for both spectral regions, a complete linelist for atmospheric applications. Indeed in common access spectroscopic databases there exists, up to now, no line parameters for the 5.7 μm region (the ν_2 band), while, at 3.6 μm (ν_1 and ν_5 bands together with nine dark bands), the quality of the line parameters is quite unsatisfactory. High-resolution Fourier transform spectra were recorded at LADIR for the whole 1600 – 3200 cm^{-1} spectral range and for different path-length-pressure products conditions. Using these spectra, a large set of H_2CO individual line intensities and of self- and N_2 -broadening linewidths were measured. For the line widths of the ν_2 transitions at 5.7 μm , Complex Robert Bonamy (CRB) calculations were performed, and the calculations and measurements were compared. The experimental intensities were least squared fitted, leading to a set of high quality intensities parameters for both spectral regions. Finally, a linelist was generated in the 5.7 and 3.6 μm regions, and for this task we used the line positions generated previously for the 5.7 μm ¹ and 3.6 μm ² regions. The calculated band intensities derived for the 5.7 μm and 3.6 μm bands are in excellent agreement with the values achieved recently by medium resolution band intensity measurements. It has to be mentioned that intensities in the 3.6 μm achieved in this work are, on the average, about 28 % stronger than those quoted in the HITRAN database. Also at 3.6 μm the quality of the individual line parameters are significantly improved as compared to our previous study performed in 2006^b.

¹F. Kwabia Tchana, A. Perrin and N. Lacome, *J. Mol. Spectrosc.*, 245, 141-144, 2007

²A. Perrin, A. Valentin and L. Daumont, *J. Mol. Struct.* 780-782, 28-44, 2006

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CONFERENCE PROGRAM

DAY 1, Sunday 22 June

7:30 Registration
9:00 WELCOME Laurence S. Rothman

SESSION I: Astrophysics

Chair: C. E. Miller

9:15 (KEYNOTE) High-Resolution Spectroscopy and Astronomical Detection of Molecular Anions S. Brünken
10:00 Characterizing Pale Blue Dots in the Sky - Spectral Fingerprints from Earth to Super-Earth L. Kaltenecker

10:30 Precise Modeling of Atmospheric Absorption Features in High-Resolution Astronomical Spectra A. Seifahrt

11:00 *Coffee Break*

Chair: I. E. Gordon

11:15 High-Accuracy Spectral Lines for Radiation Transport in Stellar Atmospheres A. Sharma
11:45 Non-linear Effects of Atmospheric Extinction on Observations in Astronomy F. Zagury
12:15 *Lunch Served*

SESSION II: Databases

Chair: P. F. Bernath

13:30 Near-Infrared Carbon Dioxide Spectral Database C. E. Miller
14:00 High Sensitivity CW-CRDS Spectroscopy of the Eight Most Abundant CO₂ isotopologues between 5851 and 7045 cm⁻¹. Critical Review of the Current Databases A. Campargue
14:30 CDSD-296 (Carbon Dioxide Spectroscopic Database): Updated and Enlarged Version for Atmospheric Applications S. A. Tashkun

15:00 Half-Widths and Line Shifts for Transitions in the ν_3 Band of Methane in the 2726 – 3200 cm⁻¹ Spectral Region for Atmospheric Applications R. R. Gamache

15:30 New Line Parameters for Near-IR Methane and the Oxygen A-Band L. R. Brown

16:00-18:00 **POSTER SESSION 1**

19:00 *Banquet*

DAY 2, Monday 23 June SESSION III: Databases-2

Chair: M. A. H. Smith

9:00 JPL Millimeter and Submillimeter Spectral Line Catalog B. J. Drouin

9:30 The IUPAC Water-Vapour Database. J. Tennyson

10:00 W@DIS: Water spectroscopy with a Distributed Information System A. Z. Fazliev

10:30 *Coffee Break*

Chair: J. Tennyson

10:45 Updated Line-List of ¹⁶O₃ in the Range 5860 – 7000 cm⁻¹ Deduced from CRDS Spectra Sensing A. Barbe

11:15 Combining HITRAN Line-By-Line, UV Cross Section and PNNL Databases for Modeling of LIBS and Raman LIDAR D. Plutov

11:45 *Lunch Served*

SESSION IV: Remote Sensing

Chair: J.-M. Flaud

13:00 Implications for Molecular Spectroscopy Inferred from IASI Satellite Spectral Measurements S. A. Clough

13:30 Improved Understanding of Far-Infrared Radiative Processes Using Measurements from the ARM North Slope of Alaska Climate Research Facility E. Mlawer

14:00 Spectrally Resolved Measurement of the Downwelling Longwave Radiance from an High-Altitude Station: Spectroscopic Issues in the Data Analysis G. Bianchini

14:30 The Atmospheric Chemistry Experiment, ACE: Latest Results P. Bernath

15:00 Spectroscopic Issues for the Atmospheric Chemistry Experiment (ACE) C. D. Boone

15:00 Applying Spectroscopy to Global Change: Isotopic Ratio Measurements of Ambient Carbon Dioxide and Methane D. D. Nelson

16:00-18:00 **POSTER SESSION 2**

DAY 3, Tuesday 24 June

SESSION V: Laboratory Spectroscopy

Chair: L. Daumont

9:00 Quantitative Measurement of Integrated Band Intensities of Benzene (C₆H₆) Vapor in the Mid-Infrared at 278, 298 and 323 K ... C. P. Rinsland

9:30 Pressure-Broadening of Water Lines in the THz Frequency Region: Improvements and Confirmations for Spectroscopic Databases C. Puzzarini

10:00 From Matrix Isolation Spectroscopy to First Observation of the CO₂ 628 Isotopologue ($\nu_2 + \nu_3$) Band in the Atmosphere Of Venus . P. R. Dahoo

10:30 *Coffee Break*

Chair: L. R. Brown

10:45 Methane for Atmospheric and Planetary Applications: What Spectroscopic Parameters Do We Need? D. Jacquemart

11:15 The High Resolution Infrared Spectrum of ³⁴SO₂ up to 4000 cm⁻¹ J.-M. Flaud

11:45 Absolute Line Intensities and Accurate Line Broadening Parameters for the 5.7 μ m and 3.6 μ m Bands of Formaldehyde A. Perrin