HITRAN-ASA

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SESSION I: Databases and Tools

I-1. Brief Report on the Status and Future Directions of the HITRAN Database

I. E. Gordon,[a] **L. S. Rothman**,[a] **Y. Tan**,[a] **R. V. Kochanov**,[a]
R. J. Hargreaves,[a] **E. K. Conway**[a]

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HITRAN2016[1] is the current official release of the database. A brief explanation of the extensions and improvements with respect to the previous compilation (HITRAN2012[2]) will be given. Some comments on the initial feedback to the database release will be given. Examples of definite improvements of the quality and extent of the spectral parameters will be demonstrated with respect to applications. Some remaining problems will also be shown and some immediate update plans will be explained.

The status and future plans for the HITEMP database[3] will also be discussed.

The HITRAN database is supported by NASA AURA and PDART program grants NNX14AI55G and NNX16AG51G.

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[1] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[2] L. S. Rothman, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 130, 4-50 (2013).

[3] L. S. Rothman, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 111, 2139-2150 (2010).

I-2. Considerations for Sharing and Preserving Research Software and Data

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Access to research software and data are foundationally important to both the future and the heritage of scientific research. Deep intellectual contributions are being made by people building software that is increasingly unable to be decoupled from data itself. Digital research artifacts like code in particular present new challenges to traditional scholarly communication models and digital preservation practices as versioning and authorship in these contexts are fluid. It is nevertheless essential that scientists are encouraged to create these valuable resources and that practices are adopted to enable people to share these complex, distributed, changing tools as easily as they share articles. A brief overview of emerging best practices in this context will be presented along with concrete actions scientists can take to make their research software and data more open, citable, and persistent to ensure the legacy of their work.

I-3. PNNL Databases for Atmospheric Monitoring

T. J. Johnson,[a] **T. L. Myers,**[a] **S. W. Sharpe,**[a] **R. L. Sams,**[a] **R. G. Tonkyn,**[a]
M. S. Taubman,[a] **T. O. Danby,**[a] **J. C. Birnbaum**[a]

[a] *Pacific Northwest National Laboratory, Richland WA, USA*

We will report technical details and content for three different PNNL infrared spectral databases that are of utility to atmospheric scientists. The first is the original Northwest infrared (NWIR) gas-phase database sponsored by DOE: This data set contains quantitative, gas-phase infrared spectra of 462 pure chemical species that can be used for a variety of applications such as atmospheric monitoring, biomass burning studies, threat detection, etc. It includes several background species as well as gases associated with various energy production cycles. The data, recorded at 0.1 cm^{-1} spectral resolution, are pressure broadened to one atmosphere (N_2) in order to mimic atmospheric conditions. Each spectrum is a composite derived from multiple (10+) individual measurements. The second database is also gas-phase and is technically identical to the first: 600 to 6500 cm^{-1} spectra recorded with gases pressure broadened to 760 Torr. This set was sponsored by SERDP and includes 62 different molecules that are known or suspected biomass-burning effluents, many being oxygenated volatile organic compounds (OVOCs). The third, more recent, database is comprised only of liquids: In this effort, sponsored by IARPA, we have derived the complex optical constants n and k for ∼60 liquids by recording a series of quantitative spectra using cells of known path lengths. Linear Beer-Lambert behavior is obtained in an iterative fashion using absorption bands of both strong and weak intensities to get consistent values for k. Based on the method of Bertie et al.[1] the real component n is then obtained using a refractometer to obtain n followed by application of the Kramers-Kronig transform. Examples from each of the three data sets will be discussed along with the experimental details, including both strengths and limitations of the experimental data.

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[1] J. E. Bertie, et al., *Appl. Spectrosc.*, 47, 1100-1114 (1993).

I-4. Spectroscopic Toolbox for HITRAN

R. V. Kochanov,[a] **I. E. Gordon**,[a] **L. S. Rothman**,[a] **Y. Tan**,[a] **C. Hill**,[b]
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In this talk we give an overview of the current state and updates of the infrastructure for the HITRAN[1] database. We will emphasize the new possibilities of data acquisition using the most recent version of the HITRAN Application Programming Interface (HAPI, the description of the first version can be found in the corresponding paper[2]) which is being developed in the HITRAN group. The HAPI toolkit is built upon the object model, which include the basic spectroscopic entities and lets the user implement the full cycle from downloading and parsing the data to obtaining complex molecular spectra by a tiny amount of Python code. This new version (HAPI v2) extends the capabilities of the HAPI both in terms of the web-access (web-API) and the code (Python SDK). The Python SDK (software development kit) is an open source project[3] which will include additional features, such as additional line profiles, instrumental functions, and line mixing. The web API extends the querying capabilities by providing the access to meta-data for sources, as well as cross-sections for more than 300 molecules through Python SDK. The graphical user interface (GUI) HAPIEST (HAPI and Efficient Spectroscopic Tools) will also be presented. The portable HAPIEST software is also available on GitHub[4] and enables the user to access the HAPI functionality without installation of Python and its libraries.

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[1] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[2] R. V. Kochanov, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 177, 1530 (2016).

[3] https://github.com/hitranonline/hapi

[4] https://github.com/hitranonline/hapiest

I-5. Evaluation of the Spectroscopic Parameters of Current Spectroscopic Databases, such as GEISA-2015 and HITRAN-2016, in the Frame of the New 2018 Release of GEISA

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The accuracy of molecular spectroscopy in atmospheric research has entered in a new phase in the frame of remote sensing applications (meteorology, climatology, chemistry) with the advent of highly sophisticated and resolved instrumentations.

The latest 2015 release of GEISA, including line parameters, cross-sections as well as aerosols, has been described in Jacquinet et al.[1]

In parallel, the corresponding line parameters have been intensively validated using the powerful approach of the SPARTE chain[2] developed at LMD. For this release, important conclusions have been obtained, especially for H_2O, CO_2 and CH_4.

GEISA and associated management software facilities are implemented and freely accessible on the AERIS/ESPRI atmospheric data center website[3]. It is used on-line in various domains like atmospheric physics, planetology, astronomy, astrophysics. GEISA line parameter database is the reference for current or planned TIR/SWIR space missions, such as for IASI, IASI-NG, MERLIN, Microcarb.

Now, at LMD, we have initiated the next release of GEISA-2018, planned for the end of this year. Using the SPARTE chain, and after a brief description of what will be the main updates waited in GEISA-2018, we will give an overview of the current status of the spectroscopy (GEISA-2015, HITRAN-2016, ...), as well as the preliminary results of the validation of the first molecules updated in GEISA-2018 such as for H_2O, CO_2, O_3, N_2O, CO and CH_4.

---

[1] N. Jacquinet-Husson, et al., *J. Mol. Spectrosc.*, 327, 31-72 (2016).

[2] R. Armante, et al., *J. Mol. Spectrosc.*, 327, 180-192 (2016).

[3] https://cds-espri.ipsl.upmc.fr/etherTypo/index.php?id=950&L=1

I-6. MODTRAN6 Line-By-Line Algorithm

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[a]*Spectral Sciences Inc, Burlington MA, USA*

A line-by-line (LBL) algorithm has been developed for use within the MODTRAN6 atmospheric radiative transfer model. The model computes both emitted and scattered line-of-sight radiances utilizing a spherical refractive geometry package and the DISORT discrete ordinate model to solve the 1-D scattering problem. The MODTRAN6 LBL method distinguishes itself from most other monochromatic models in that the radiative transfer problem is solved at arbitrarily fine spectral resolution within disjoint and contiguous 0.1 cm^{-1} steps, marching through the user-specified band pass. The advantage of this approach is that the predominantly Lorentzian, temperature and pressure dependent contributions to each 0.1 cm^{-1} spectral bin from molecular transitions centered more than 0.05 cm^{-1} from the bin can be summed off-line and fit to a simple analytic form. The line-shape of each molecular transition is explicitly modeled on-the-fly only over a narrow 0.2 cm^{-1} sub-region. The challenge of this approach is to ensure that spectral discontinuities do not arise at spectral bin edges, where the method for modeling absorption from individual molecular lines changes abruptly. Interpolations based on the radiative transfer physics of the pre-computed line tail data are introduced to produce a smooth transition across these edges. Spectral validations against LBLRTM verify the fidelity of the approach. The new MODTRAN LBL algorithm is used to quantify the accuracy of the MODTRAN band model and correlated-k statistical approaches under varying conditions.

I-7. Spectroscopic Databases for the VAMDC Portal: New Tools and Improvements

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Dijon spectroscopic databases include calculated line lists, in positions and intensities, that are obtained from experimental spectroscopic analyses. They contain 6 molecules: CH_4, C_2H_4, CF_4, SF_6, GeH_4 and RuO_4 and are all compatibles with the XSAMS (XML Schema for Atoms, Molecules, and Solids) format adopted with the Virtual Atomic and Molecular Data Centre (VAMDC) Project. VAMDC, the worldwide consortium which federates atomic and molecular databases through an e-science infrastructure, aims to provide a unique access point for scientists seeking the best atomic and molecular data for their studies. So far, development of new tools allows to easily download and compare data issued from different databases in a single XML document or into the HITRAN2004 format. Making the comparison that easy will help data users in the choice of data that best match their needs. It will also help data producers by checking the consistency of their data.

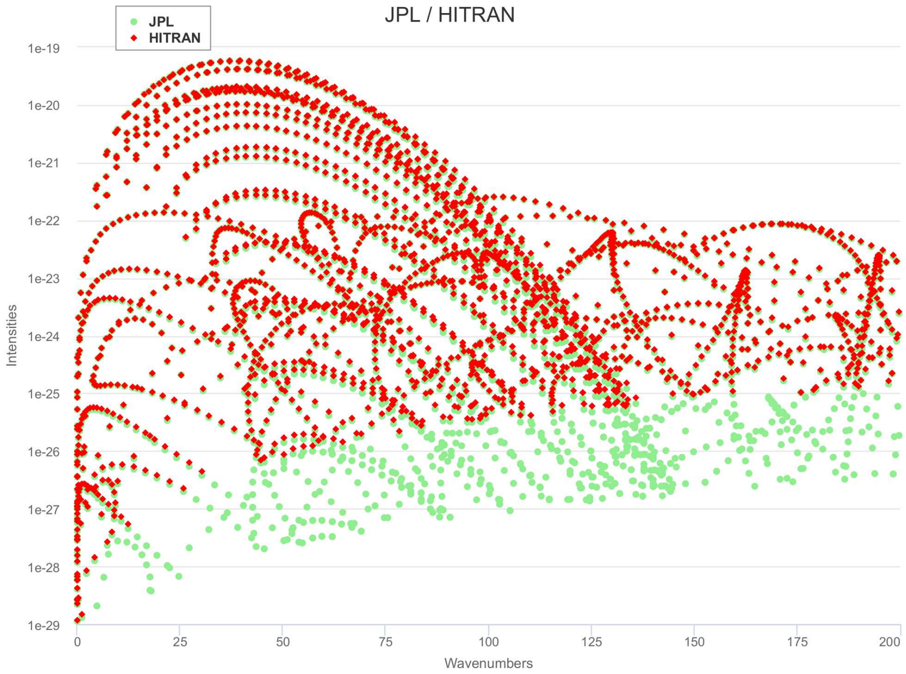

Figure 1

SESSION II: Planetary-Relevant and High-Temperature Spectroscopy

High Temperature Laboratory Measurements, Atmospheric Retrievals, and Future Plans for HITEMP

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This talk will overview my research in the field of spectroscopy. The first section will discuss the motivations and observations of high temperature empirical line lists, with emphasis on NH_3 and CH_4, and how recent collaborations have combined both theoretical and experimental methods to extend assignments and improve calculations. Furthermore, for heavier molecules (e.g., C_2H_6) the challenge of producing line lists is exacerbated at high temperatures, therefore experimental cross-sections have been measured.

Next there will be a brief excursion into atmospheric retrievals of NH_3 from nadir viewing, hyperspectral sounding instruments (e.g., IASI). Full optimal estimation retrievals require large processing times, hence fast retrieval methods are required for near-real time measurements. This talk will introduce the scaled linear retrieval technique, which aims to provide a better estimate for the total column of tropospheric species (e.g., NH_3) while remaining fast to compute.

Finally, the latest developments toward the upcoming release of HITEMP[1] will be discussed. The current version of HITEMP contains five molecules (i.e., H_2O, CO_2, CO, NO, and OH), however some molecules omitted due to limited or inaccurate high temperature data, have now become important for the characterization of exoplanets, cool stars and brown dwarfs (e.g., CH_4). The next major update of HITEMP will be discussed, with a brief description of the aims and difficulties that will need to be addressed.

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[1] L. S. Rothman et al., *J. Quant. Spectrosc. Radiative Transf.*, 111, 2139-2150 (2010).

II-2. Frequency Comb Lasers in High-Temperature Spectroscopy: Spectral Database Development to Practical Field Measurements

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Frequency combs are a unique class of lasers that emit hundreds to hundreds of thousands of distinct, equally-spaced wavelength elements ('comb teeth'). Dual comb spectroscopy (DCS) is a method for absorption spectroscopy that uses massively parallel heterodyne detection between two frequency combs with slightly different tooth spacing. When used with mode-locked frequency comb lasers, DCS is unique in its ability to resolve the absorption on each comb tooth across a very wide spectral bandwidth using a single high-speed photodetector. Recent advances in robust frequency comb technology have enabled mobile DCS applications for the first time[1], including for measurements of temperature and species concentrations in high-temperature environments[2]. The success of broadband, high-resolution absorption spectroscopy at high temperatures depends on good underlying spectral databases providing accurate models of high-temperature molecular absorption which can be used to fit data from unknown environments.

We present an overview of recent work to apply DCS to high-temperature environments. Specifically, we develop a spectral database for water vapor absorption from 6800 cm^{-1} to 7190 cm^{-1} using a carefully-controlled tube furnace at temperatures up to 1300 K and advanced multispectral fitting techniques[3]. The dataset and multispectral fitting approach provide an excellent opportunity to test the ability of different lineshapes to model high-temperature water vapor lineshapes[4]. We apply the new database for field measurements of temperature in a coal gasification system, and discuss new directions for the technology in high-temperature environments.

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[1] S. Coburn, et al., *Optica*, 5, 320 (2018).

[2] P. Schroeder, et al., *Proceedings of the Combustion Institute*, 36, 4565 (2017).

[3] P. Schroeder, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 210, 240 (2018).

[4] P. Schroeder, et al., *Physical Rev. A*, 96, 022514 (2017).

II-3. Laboratory Spectroscopy for Exoplanets

P. F. Bernath [a]

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Recent results from our laboratory will be surveyed on the analysis of TiO spectra and preparation of line lists for NH, OH, OH^+ using experimental measurements with a Fourier transform spectrometer for line positions and *ab initio* dipole moment functions for line intensities. Our measured cross sections and line lists for high temperatures for small polyatomic molecules such as methane and ammonia will also be presented as well as measurements of infrared absorption cross-sections for small hydrocarbons.

II-4. Line Positions and Intensities for the ν_3 Band of 5 Isotopologues of Germane for Planetary Applications

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Germane (GeH_4) is present in the atmospheres of the giant planets Jupiter and Saturn. The ongoing NASA mission Juno has renewed interest in its spectroscopy. The accurate modeling of which is essential for the retrieval of other tropospheric species. We present here the first complete analysis and modeling of line positions and intensities in the strongly absorbing ν_1/ν_3 stretching dyad region near 2100 cm^{-1}, for all five germane isotopologues in natural abundance[1]. New infrared spectra were recorded, absolute intensities were extracted through a careful procedure and modeled thanks to the formalism and programs developed in Dijon. A database of calculated germane lines, GeCaSDa, is available online through the Virtual Atomic and Molecular Data Centre (VAMDC) portal[2] and at http://vamdc.icb.cnrs.fr/PHP/gecasda.php. GeH_4 will be added the HITRAN database.

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[1] V. Boudon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 205, 174–183 (2018).

[2] http://portal.vamdc.org

II-5. Water Vapor: Line Intensity Study of ^{18}O Enriched Spectra Between 6450 and 8000 cm^{-1} and H_2O Line Shape Parameters Broadened by CO_2

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This presentation will focus on two subjects, in a first part the study of $H_2{}^{18}O$ line intensities around 1.3 μm and in a second part, the line-shape parameters of H_2O in collision with CO_2 in the spectral regions of 2.7 and 6 μm. All high-resolution spectra were recorded in the GSMA laboratory with the Connes-type Fourier Transform Spectrometer[1] at room temperature.

The spectrum analysis of ^{18}O enriched water vapor absorption between 6450 and 9300 cm^{-1} is in progress, using the same procedure as that performed previously in the same spectral region but for the main isotopologue[2]. Overall, more than 3000 absorption lines of six water isotopologues ($H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, $HD^{16}O$, $HD^{17}O$ and $HD^{18}O$) were observed. Among them, about 300 lines correspond to the transitions of previously unknown upper energies of $H_2{}^{18}O$ and $H_2{}^{17}O$. Some examples of the disagreements between experimental spectra and the simulations using HITRAN2016 line list[3] in the spectral region between 6450 and 8000 cm^{-1} will be presented and discussed.

In a second part, new results on the line-shape parameters of H_2O lines broadened by CO_2 will be presented. Considering the resolution of nowadays remote instruments, accurate knowledge of line shape parameters of H_2O in CO_2 could be important for the study of CO_2-rich atmospheres like those of Mars and Venus. New measurements of CO_2-broadened H_2O line widths and shifts around 2.7 and 6 μm as well as comparisons with literature[4,5] will be presented.

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[1] L. Régalia, X. Thomas, S. N. Mikhailenko, 13th ASA Conference (united with 14th HITRAN Conference). 2016. August 24-26. Reims. France.

[2] L. Régalia, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 136, 119-136 (2014).

[3] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[4] L. R. Brown, et al., *J. Mol. Spectrosc.*, 246, 1-21 (2007).

[5] Y. G. Borkov, et al., *J. Mol. Spectrosc.*, 344, 39-45 (2018).

II-6. Line Positions and Intensities in the 7400−8600 cm^{-1} Region of the Ammonia Spectrum

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The positions and intensities of 1936 lines observed in the range 7400 − 8600 cm^{-1} of two absorption spectra of ammonia recorded at high resolution using Fourier transform spectroscopy are reported. The accuracy of these line positions is estimated to range from 0.001 to 0.002 cm^{-1} from the lower to the upper limits of the spectral range considered, while the accuracy of the line intensities is estimated to be around 10% or better. Also reported are less-accurately measured positions and intensities of 1985 lines retrieved from these two spectra or from only one of them. These results are compared with the data measured recently in a spectrum recorded in 1980 at the Kitt Peak National Solar Observatory[1] and provided in HITRAN 2016, as well as line positions and intensities measured in this work in the same Kitt Peak spectrum.

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[1] E. J. Barton, et al., *J. Mol. Spectrosc.*, 325, 7-12 (2016).

Poster Session

P-1. New Measurements of the Water Vapor Absorption Cross Section in the Blue-Violet Range by Cavity-Enhanced Differential Optical Absorption Spectroscopy

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The absorption cross section of water vapor in the blue-violet range (415–460 nm) is currently not well known, and many weak spectral lines are not included in either the HIgh resolution TRANsmission molecular absorption (HITRAN) database or its HIgh TEMPerature companion, HITEMP. Direct measurements of the absorption cross section of water vapor in this region have been limited by the slant column density (SCD) of gaseous water molecules that is achievable in a laboratory setting. We use cavity-enhanced differential optical absorption spectroscopy (CE-DOAS) to generate water vapor SCDs comparable to those in remote sensing field measurements under well controlled laboratory conditions. A pair of high-reflectivity ($R > 0.99995$) mirrors are separated by $\sim$80 cm to realize effective path lengths up to 16 km; water vapor is generated from deionized water in a double-bubbler system. Broadband light sources (e.g. an LED with a peak intensity at 455 nm) are used to measure multiple lines at moderately high spectral resolution (0.15 nm). The first spectra were measured at room temperature (298 K), and we are now taking measurements at higher temperatures using an insulated heat exchanger system around the optical cavity. Our goal is to refine available line lists for gas-phase water by combining laboratory measurements with quantum chemical calculations; the mismatch between measured and calculated cross sections is identified as residual structures, and used to improve the calculations. We also compare the cross sections to field measurements of water in pristine air over remote oceans, i.e., in scattered solar light limb spectra in the lower tropical free troposphere that were recorded by Airborne DOAS aboard the NSF/NCAR GV aircraft during the Tropical Ocean tRoposphere Exchange of Reactive halogen species and Oxygenated VOC (TORERO) experiment.

P-2. A Highly Accurate *Ab Initio* Dipole Moment Surface for Water: Transitions Extending Into the Ultraviolet

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We present a new *ab initio* dipole moment surface (DMS) for the water molecule valid for transitions which stretch into the near ultraviolet. Intensities computed using this surface agree very well precise laboratory measurement designed to aid atmospheric observations. This work is based on a data set encompassing 17,628 multi-reference configuration interaction configurations that were calculated with the aug-cc-pCV6Z basis set with the Douglass-Kroll-Hess Hamiltonian to second order and required approximately 116 years of CPU running time to complete.

Compared to recent experimental measurements in the far infrared region[1], this new DMS significantly improves agreement with theory for transitions in the previously problematic bands (121), (300) and (102). For highly energetic overtones located in both the visible and ultraviolet regimes, we successfully predict the intensity of all measured bands to within 10% of the latest atmospheric observations[2]. These include bands at 487 nm (303), 471 nm (511), and 363 nm (900), for which previous models underestimated the intensity by up to 139%. Absorption features are also predicted in the 290 nm to 355 nm window and the theoretical shape demonstrates reasonably good behaviour with previously measured cross sections. The 10 ν_1 band is identified as the strongest absorber in this region and the maximum intensity is approximately 6.3×10^{-27} cm molecule^{-1}, which should be observable in atmospheric spectra.

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[1] M. Birk, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 88-102 (2017).
[2] J. Lampel, et al., *Atmos. Chem. Phys.*, 17, 1271-1295 (2017).

P-3. Comparison of Different Water Vapour Absorption Line Lists to Measured Atmospheric Absorptions using Ground-Based MAX-DOAS Observations

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M. Yang,[e] **M. Horbanski,**[a,b] **S. Schmitt,**[a] **U. Frieß,**[a] **T. Wagner,**[f] **U. Platt**[a,b,f]

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Water vapour absorptions can be found from the microwave to the near ultraviolet spectral region. They overlay the absorption structures of a number of other trace gas species. Precise knowledge of the water vapour absorption cross-section can therefore be crucial for precise spectroscopic measurements of various other trace gases in the Earth's atmosphere, such as e.g., NO_2, O_3, HONO, O_4, IO and Glyoxal. Based on absorption spectra measured by ground-based MAX-DOAS instruments at medium spectral resolution (typically 0.5 nm), we present an assessment of how well present water vapour absorption line lists represent measured absorptions in the Earths atmosphere in different spectral regions from 333 nm (30,000 cm^{-1}) to 570 nm (17,500 cm^{-1}). These measurements were done in the course of a whole year at the south coast of England and thus provide measurements at different absolute humidities. We compare the line lists HITRAN 2008, HITRAN 2012 / HITEMP, HITRAN 2016, BT2 and POKAZATEL. We show that recent *ab initio* absorption spectra represent water vapour absorption increasingly well. For the UV spectra range we could show before that certain line lists predict the shape and wavelengths of water vapour absorption bands quite well. In this presentation we now show that recent improvements increase also the agreement in the blue spectral regions, where previously differences in the magnitude of more than 50% were reported. We use the MAX-DOAS measurements to compare them the measured absorption structures to currently available water vapour line lists in order to provide a quantitative measure of their agreement with atmospheric observations. In this study we also estimate potential cross-interferences of the respective water vapour absorption line list on the retrieved amount of tropospheric absorbers of interest. In the blue spectral range, differences between NO_2 evaluations of up to 5×10^{15} molec cm^{-2}

were observed under mid-latitude summer conditions using the listed line lists above. This corresponds to about 0.2 ppb of NO_2 for a light path length of 10 km. This is significant for measurements in pristine regions. Significant differences are also found for IO, glyoxal and other compounds. These findings are therefore of interest for the spectral retrieval of various atmospheric absorbers measured by any type of DOAS setup.

P-4. Validation of Non-Voigt Line Shape Function in Tunable Diode Laser Absorption Spectroscopy of Water Vapor at 1390 nm

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The validity of non-Voigt line shape functions was investigated by using tunable diode laser absorption spectroscopy (TDLAS) of water vapor at 1390 nm. Water vapor was contained in Brewster-angled quartz cell ($l \sim$ cm). Optical layout was fully fiber coupled. A branch of the DFB laser was fed to an optical spectrum analyser in order to calibrate wavelength. Fiber coupled InGaAs photodiode detected a transmitted laser power. Laser wavelength was modulated at ~60 Hz of symmetric triangular function. Since a laser power was modulated meantime, a modulation depth of the DFB laser was optimized to secure full vertical resolution of 12-bit oscilloscope of which sampling rate was around 50 Ms/sec. In order to generate absorption spectra, background lines were fitted by third order polynomial of which validity was ensured by separated measurement with dummy cell. Absorption line shapes were fitted by reduced functions from Hartman-Tran functions such as Voigt, Rautian, Speed Dependent Voigt, and Speed Dependent Rautian functions. Source code of the Hartman-Tran function in the HAPI code written by the PYTHON was abstracted and translated to the MATLAB in order for implementation to our own code. The Galatry function was formulated based on the hypergeometric function. To fit the experimental line shapes, a Levenberg-Marquardt algorithm was used. Our code will be extended to perform forward and inverse modeling of high-resolution spectra measured by various spectroscopic techniques including high resolution FTIR, cavity ringdown (or enhanced) spectroscopies. The fitting results of spectra measured at 2.5 Torr and room temperature showed best result with SD-Voigt. Global standard deviation of residual was 4.89×10^{-4}. This suggests that speed dependence due to inelastic collision should be considered when considering self broadening. Our research will be improved to provide SI-traceable oscillator strengths and broadening coefficients.

P-5. Vibrational Dependence and Prediction of Line Shape Parameters for the H_2O-H_2 Collisional System

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The Modified Complex Robert-Bonamy (MCRB) formalism was used to calculate the half-width, γ, and line shift, δ, for the H_2O-H_2 collision system at 14 temperatures between 200 and 3000 K for over 7 thousand rotational transitions for the rotation band, the (301)-(000) band and bands for ν_1, ν_2, and ν_3 with 1-4 vibrational quanta exchanged. These data were used to study the vibrational dependence of the half-width and line shift. It is shown that the H_2O-H_2 collision system is strongly off-resonance. The results demonstrate strong and unusual vibrational dependence.

The half-width and line shift data for different vibrational bands were used to determine if a prediction routine for γ and δ could be developed. Following the work of Jacquemart et al.[1] and Gamache and Lamouroux[2], the expressions

$$\gamma\left[\left(\nu_1^{'},\nu_2^{'},\nu_3^{'}\right)f \leftarrow \left(\nu_1^{''},\nu_2^{''},\nu_3^{''}\right)i\right] = I^{\gamma}_{f\leftarrow i} + A_{f\leftarrow i}\left(c_1\left|\Delta\nu_1\right| + c_2\left|\Delta\nu_2\right| + c_3\left|\Delta\nu_3\right|\right)^{p_\gamma}$$

and

$$\delta\left[\left(\nu_1^{'},\nu_2^{'},\nu_3^{'}\right)f \leftarrow \left(\nu_1^{''},\nu_2^{''},\nu_3^{''}\right)i\right] = I^{\delta}_{f\leftarrow i} + B_{f\leftarrow i}\left(c_1\left|\Delta\nu_1\right| + c_2\left|\Delta\nu_2\right| + c_3\left|\Delta\nu_3\right|\right)^{p_\delta}$$

were used to predict the half-width and line shift where the powers p_γ, p_δ, and coefficients $I^{\gamma}_{f\leftarrow i}$, $A_{f\leftarrow i}$, $I^{\delta}_{f\leftarrow i}$, and $B_{f\leftarrow i}$ were determined by non-linear least-squares techniques. In addition, a normal mode prediction technique was also studied.

The results of the fits are discussed in the context of this unusual collision system.

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[1] D. Jacquemart, R. R. Gamache, L. S. Rothman, *J. Quant. Spectrosc. Radiat. Transf.*, 96, 205-239 (2005).

[2] R. R. Gamache, J. Lamouroux, *J. Quant. Spectrosc. Radiat. Transf.*, 130, 158-171 (2013).

P-6. *Ab Initio* Reduced Matrix Elements for $H_2{}^{16}O$ for Modified Complex Robert-Bonamy Calculations

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The determination of the reduced matrix elements (RMEs) is an important part of the Modified Complex Robert-Bonamy (MCRB) calculations. Lamouroux et al.[1] used *ab initio* wavefunction of Partridge and Schwenke[2] to determine the RMEs and derived sums rules on RMEs, based on physical properties, to check the calculated RMEs.

In this work, the sums rules have been applied to the RMEs of a number of vibrational states. For many rotational states the sum rules are obeyed, however for many others they do not give the correct sum. The use of incorrect RMEs is a source of inaccuracy in the MCRB calculations that can significantly affect the determination the collisional half-width and the line-shift. Calculation using the ground state and the vibrational dependent RMEs were performed to show the influence of this spectroscopic effect.

In order to understand this spectroscopic effect, RMEs computed for different vibrational states were compared to the ground state values. The differences were related to the symmetry, oblateness/prolateness, and Ma rule paring of the *ab initio* H_2O wavefunctions.

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[1] J. Lamouroux, R. R. Gamache, D. W. Schwenke, *J. Quant. Spectrosc. Radiat. Transf.*, 148, 49-57 (2014).

[2] H. Partridge, D. W. Schwenke, *J. Chem. Phys.*, 106, 4618-39 (1997).

P-7. Line Intensities of the 30011e − 00001e Band of $^{12}C^{16}O_2$ with Laser-Locked Cavity Ring-Down Spectroscopy

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Thirty well isolated ro-vibrational transitions of the 30011e − 00001e band of $^{12}C^{16}O_2$ at 1.54 μm have been recorded with a laser-locked cavity ring-down spectrometer. The line intensities were obtained with accuracies better than 0.85%. Comparisons of the line intensities determined in this work with literature experimental values[1] and those from HITRAN2016[2], AMES[3], UCL-IAO[4] and CDSD-296[5] line lists are given.

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[1] R. A. Toth, et al., *J. Mol. Spectrosc.*, 239, 221-242 (2006).

[2] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[3] X. C. Huang, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 224-241 (2017).

[4] E. Zak, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 177, 31-42 (2016).

[5] S. A. Tashkun, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 152, 45-73 (2015).

P-8. Laser Spectroscopy Monitoring of $^{13}C^{18}O^{16}O$ and $^{12}C^{17}O^{16}O$ of Atmospheric Carbon Dioxide

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One of the main challenges to making accurate predictions of future changes in carbon dioxide (CO_2) concentration is the capability to determine what fraction of human produced CO_2 remains in the atmosphere. We present our progress in the application of Tunable Infrared Laser Direct Absorption Spectroscopy (TILDAS) to the measurement of the primary clumped ($^{13}C^{18}O^{16}O$) as well as ^{17}O ($^{12}C^{17}O^{16}O$) isotopologues of atmospheric CO_2, as a tracer of its sources and sinks. We expect unique isotopologue signals in CO_2 from high-temperature combustion sources, plants, soils, and air-sea exchange processes. High sampling frequency (a few minutes for each sample vs. reference cycle) achieved by a TILDAS instrument is expected to enable us to document local heterogeneous sources and temporal variations.

The TILDAS is equipped with a 400-meter optical absorption cell which provides sufficient sensitivity for direct measurements of the rare clumped isotopologue. We designed a dual pressure measurement technique in which the clumped isotopologue, $^{13}C^{18}O^{16}O$, and $^{13}C^{16}O^{16}O$ are first measured at $\sim$25 Torr cell pressure. This is followed by measurement of $^{12}C^{17}O^{16}O$, $^{12}C^{18}O^{16}O$ and $^{12}C^{16}O^{16}O$ at lower ($\sim$2 Torr) cell pressure. Isotopologue ratios are compared between reference and sample gases. We demonstrated a precision approaching 0.03‰ for the ratio $^{13}C^{18}O^{16}O/^{13}C^{16}O^{16}O$ and 0.08‰ for $\Delta^{13}C^{18}O^{16}O$ value (1σ repeatability for 4 min sample vs. reference cycle). Sample size for a single analysis is approximately 100 mL of air (1.6μmol of CO_2). Given the previously observed range of variations for $\Delta^{13}C^{18}O^{16}O$ and $\Delta^{17}O$ in atmospheric samples (as large as 0.6 to 0.3‰, respectively), TILDAS offers the possibility of real time, nearly continuous monitoring of these signals.

Achieving better than 0.1‰ precision requires careful matching of CO_2 mixing ratios between reference and sample air. A primary cause of pressure and mixing ratio dependence is inaccurate baseline fitting analogous to abundance sensitivity or pressure baseline for IRMS). Given that mixing ratios of atmospheric carbon dioxide can vary as much as 50% or more, a dynamic dilution scheme, where sample air is diluted by CO_2 free air to match the reference mixing ratio, is being developed. An in-line calibration source of hot, equilibrated CO_2 isotopologues is also being tested. We will discuss the current instrument performance, areas for improvement, and project future applications.

P-9. Consistency of Absolute Ozone Intensities in MW, 10 and 5 Micron Ranges from *Ab Initio* Predictions and Laboratory Observations

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The problems of the consistency of the ozone intensity data of the ozone molecule in various spectral infrared regions including 10 μm, 5 μm and the UV cross-sections has been subject of many discussion in the past decades but is not yet completely solved[1,2,3,4,5,6]. We present *ab initio* calculations for absolute line intensities in the most important absorption regions: in the microwave (rotational transitions) in the 10 micron range (stretching fundamentals) and in the 5 micron range (first triad of stretching overtone and combination bands) using our potential energy[6] and dipole moment[7] surfaces. The estimated intensity accuracy of our theoretical list is expected to be about 1% or even better. Our *ab initio* predictions will be compared to the recent yet unpublished FTS measurements of GSMA Reims group covering the ranges 800–2300 cm^{-1} as well as to existing databases (S&MPO[8], HITRAN[9], GEISA[10], JPL[11]). Origins of various error sources and data inconsistencies will be discussed. We acknowledge the support from LEFE CHAT CNRS French program and from Mendeleev funding TSU grant.

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[1] J.-M. Flaud, et al., *J. Geophys. Res.*, 108, 4269 (2003).

[2] B. Picquet-Varrault, et al., *J. Phys. Chem. A*, 109, 1008 (2005).

[3] M. A. Smith, et al., *J. Quant. Spectrosc. Radiative Transf.*, 113, 825 (2016).

[4] J. Orphal, et al., *J. Mol. Spectrosc.*, 327, 105 (2016).

[5] C. Janssen, et al., *J. Mol. Spectrosc.*, 326, 48 (2016).

[6] Vl. Tyuterev, et al., *J. Chem. Phys.*, 139, 134307 (2013).

[7] Vl. Tyuterev, R. Kochanov, S. Tashkun, *J. Chem. Phys.*, 146, 064307 (2017).

[8] Y. Babikov, et al., *J. Quant. Spectrosc. Radiative Transf.*, 145, 169 (2014).

[9] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[10] N. Jacquinet-Husson, et al., *J. Molec. Spectrosc.*, 112, 2395 (2016).

[11] J. Pearson, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 111, 1614 (2010).

P-10. Isotopic Effects in Infrared Spectra of Phosphine (PH_3) and Hydrocarbons (CH_4, C_2H_4) via *Ab Initio* and Variational Calculations

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Isotopic substitutions as H → D or even $^{12}C \rightarrow {}^{13}C$ have substantial consequences on molecular spectra. To interpret correctly the experimentally observed spectra of molecules in their natural abundances, it is essential to have realistic and reliable theoretical models.

There is much less information on assigned experimental spectra of rare isotopologues, particularly for the intensities. The corresponding line lists at medium spectral resolution could be provided by the *ab initio* theory and global nuclear motion variational calculations.

The aim of this work will be to study the effects of isotopic substitutions in PH_3, CH_4, and C_2H_4, on both line positions and line intensities, from nonlinear transformations and symmetry considerations. In case of phosphine we consider PH_2D, PHD_2 isotopologues[1], and $^{12}C \rightarrow {}^{13}C$ substituted species for the methane and the ethylene. All calculations are based on our recent *ab initio* potential and dipole moment surfaces[2,3,4,5,6,7] using variational normal mode calculations[8,9]. The corresponding line lists will be made available via the TheoReTS information system[10,11,12].

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[1] D. Viglaska, et al., to be submitted.

[2] A. Nikitin, et al., *J. Chem. Phys.*, 131, 244312 (2009).

[3] A. Nikitin, et al., *Chem. Phys. Lett.*, 565, 5 (2013).

[4] T. Delahaye, et al., *J. Chem. Phys.*, 141, 104301 (2014).

[5] T. Delahaye, et al., *Chem. Phys. Lett.*, 639, 275 (2015).

[6] A. Nikitin, et al., *J. Chem. Phys.*, 145, 114309 (2016).

[7] A. Nikitin, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 200, 90 (2017).

[8] M. Rey, et al., *J. Chem. Phys.*, 141, 044316 (2014).

[9] M. Rey et al., *J. Chem. Phys. A*, 119, 4763 (2015).

[10] M. Rey, A. Nikitin, Y. Babikov, V. Tyuterev, *J. Mol. Spectrosc.*, 327, 138 (2016).

[11] http://theorets.univ-reims.fr

[12] http://theorets.tsu.ru

P-11. Atlas of Experimental and Theoretical High-Temperature Methane Cross-Sections from T=296 K to 1000 K

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Spectra of hot methane were recorded at Old Dominion University using a tube furnace, a quartz cell (optical path length of 50 cm) and a Bruker 120/125 HR spectrometer. For each temperature, a total of 600 interferograms were recorded for both the sample and corresponding background at a resolution of 0.02 cm^{-1}. The experimental setup is similar to that in Hargreaves et al.[1] In the present work, we obtained experimental absorption spectra at eight temperatures T = 296 K, 400 K, 500 K, 600 K, 700 K, 800 K, 900 K and 1000 K. These experimental records cover the near infrared range from 5400 to 9000 cm^{-1}. We have converted these into an atlas of absorption cross-sections at each temperature for the methane Tetradecad, Icosad and Triacontad polyads, excluding some particular spectral intervals strongly contaminated by water. On the theoretical side, the spectra were simulated from the *ab initio*-based Reims-Tomsk line list for the same experimental conditions. This line list has been constructed by global variational calculations from potential energy and dipole moment surfaces followed by empirical line position corrections deduced from previously published cold temperature analyses as described in Nikitin et al.[2] and Rey et al.[3,4] (and references therein). The comparisons showed very good overall agreement between observations and theory at least at medium spectral resolution. Preliminary assignments resulted in identifications of more than 10000 lines for each temperature. A full set of the theoretical absorption cross-sections is also included in the atlas. The data should be of major interest for the interpretation of current and future astronomical observations[5].

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[1] R. J. Hargreaves, P. F. Bernath , J. Bailey, M. Dulick, *Astrophys. J.*, 813, 12 (2015).

[2] A. V. Nikitin, M. Rey, V. G. Tyuterev, *J. Quant. Spectrosc. Radiat. Transf.*, 200, 90-99 (2017).

[3] M. Rey, A. V. Nikitin, V. G. Tyuterev, *Astrophys. J.*, 847, 105 (2017).

[4] M. Rey, A. V. Nikitin, Y. Babikov, Vl. G. Tyuterev, *J. Molec. Spectrosc.*, 327, 138-158 (2016).

[5] P. F. Bernath, *Phil. Trans. R. Soc. A*, 372, 20130087 (2014).

P-12. Preliminary Analysis of the Interacting $(\nu_2 + 2\nu_4,\ \nu_2 + \nu_3,\ 4\nu_2,\ \nu_1 + 2\nu_2,\ 2\nu_1)$ Pentad of CF_4

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Tetrafluoromethane CF_4 is a very powerful and long living greenhouse gas. Because of its chemical stability the lifetime of CF_4 in the atmosphere is estimated as more than 50,000 years[1]. This molecule has both natural and anthropogenic origin. It is released predominantly during aluminum refining and semiconductor manufacturing[2] into the atmosphere in significant quantities. Consequently the knowledge of the infrared spectrum of this molecule is essential for atmospheric measurements.

Experiment spectra of CF_4 in the region 1600–1800 cm^{-1} have been recorded in the GSMA Laboratory of the University of Reims Champagne-Ardenne using a Fourier transform Spectrometer of Connes type coupled to a multi-pass cell at 295 K with a spectral resolution of 0.003 cm^{-1}. All spectrum analyses and fits have been realized using the MIRS software[3] based on tetrahedral tensorial formalism. In addition, direct predictions have been made possible using full *ab initio* ro-vibrational normal mode predictions[4] and non-empirical contact transformation Hamiltonians[5,6]. We are able to perform a simultaneous fit of effective Hamiltonian parameters of several cold and hot bands of CF_4. Hamiltonian operator was expanded up to the sixth order for the ground state and for the $(\nu_2+2\nu_4,\ \nu_2+\nu_3,\ 4\nu_2,\ \nu_1+2\nu_2,\ 2\nu_1)$ pentad. Line assignments are made up to $J = 70$ and line positions are fitted with a global root mean square deviation of 1.616×10^{-3} cm^{-1} while line intensities were watched directly to those predicted by the *ab initio* variational calculations.

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[1] R. A. Morris, et al., *J. Geophys. Res. D*, 100, 1287 (1995).

[2] M. A. K. Khalil, et al., *Environ. Sci. Technol.*, 37, 4358 (2003).

[3] A. V. Nikitin, M. Rey, J.-P. Champion, Vl. G. Tyuterev, *J. Quant. Spectrosc. Rad. Transf.*, 113, 1034 (2012).

[4] M. Rey, A. V. Nikitin, V. Tyuterev, *J. Mol. Spectrosc.*, 327, 138 (2016).

[5] Vl. G. Tyuterev, et al., *SPIE Proc.*, 5311, 165 (2004).

[6] Vl. G. Tyuterev, et al., *J. Phys. Chem. A*, 117, 13779 (2013).

P-13. Line Positions and Intensities for the ν_6 and $2\nu_3$ Bands of Methyl Iodide ($^{12}CH_3I$)

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The goal of this study is to determine for the first time line positions and absolute line intensities for the ν_6 and $2\nu_3$ bands of methyl iodide ($^{12}CH_3I$) centered near 893 and 1060 cm^{-1}, respectively. High-resolution Fourier transform spectra were recorded in the 500 to 1450 cm^{-1} spectral range at various pressure–pathlength products. Using these spectra, a large set of $^{12}CH_3I$ individual line intensities was measured for the ν_6 band and least squares fit to derive the expansion of the ν_6 transition moment operator. For both line positions and intensities, the theoretical model accounts for the hyperfine structure in the 6^1 and ground states and for the vibration-rotation resonances that couple together the 6^1 energy levels with those of the 3^2 and 2^1 vibrational states[1]. As the $2\nu_3$ band is extremely weak, its associated transition moment operator was estimated from band strength values collected from the literature. In this way, a comprehensive list of line positions and intensities was generated at 10 μm for the ν_6 and $2\nu_3$ bands of CH_3I. This list could be used to help for the detection of this species in the atmosphere by the future IASI-NG satellite mission[2].

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[1] A. Perrin, et al., *J. Mol. Spectrosc.*, 324, 28-35 (2016).

[2] https://iasi-ng.cnes.fr/en/IASI-NG/index.htm

P-14. The Experimental Pure Rotational Spectrum of Some Substituted Nitrogen Hydrides. New Lines and Accurate Analyses for $^{15}ND_2$, ^{15}ND and ^{15}NH

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The pure rotational spectra of the amidogen radical $^{15}ND_2$ and of the imidogen radicals ^{15}ND and ^{15}NH were recorded by a millimetre- and a submillimetre-wave spectrometer up to the THz region.

This work represents the first experimental laboratory detection of both $^{15}ND_2$ and ^{15}ND. In the case of the amidogen radical, the analysis of the data provided a large set of rotational, electron spin-rotation and hyperfine terms. In the case of ^{15}ND, our transitions were merged with the already existing data for NH, ND and ^{15}NH and analysed in a multi-isotopologue Dunham-type fit. As far as ^{15}NH is concerned, the $N = 1 \leftarrow 0$ transition, for which just one fine-structure component was known[1], was detected around 1 THz.

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[1] S. Bailleux, et al., *Astron. Astrophys.*, 538, A135 (2012).

P-15. Update of the HITRAN Collision-Induced Absorption Section

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Correct parametrization of the Collision-induced Absorption (CIA) phenomena is essential for accurate modelling of the diverse planetary atmospheres. The HITRAN spectroscopic database provides these parameters in a dedicated section. Here we significantly revise and extend the HITRAN CIA data with respect to the original effort described in Richard et al.[1] The extension concerns new collisional pairs as well as wider spectral and temperature ranges for the existing pairs. Some of the data were replaced with new superior results. The database now contains CIA for N_2-N_2, N_2-H_2, N_2-H_2O, N_2-CH_4, N_2-O_2, O_2-O_2, O_2-CO_2, CO_2-CO_2, H_2-H_2, H_2-He, H_2-CH_4, H_2-H, H-He, CH_4-CH_4, CH_4-CO_2, CH_4-He and CH_4-Ar collision pairs. We continue to provide

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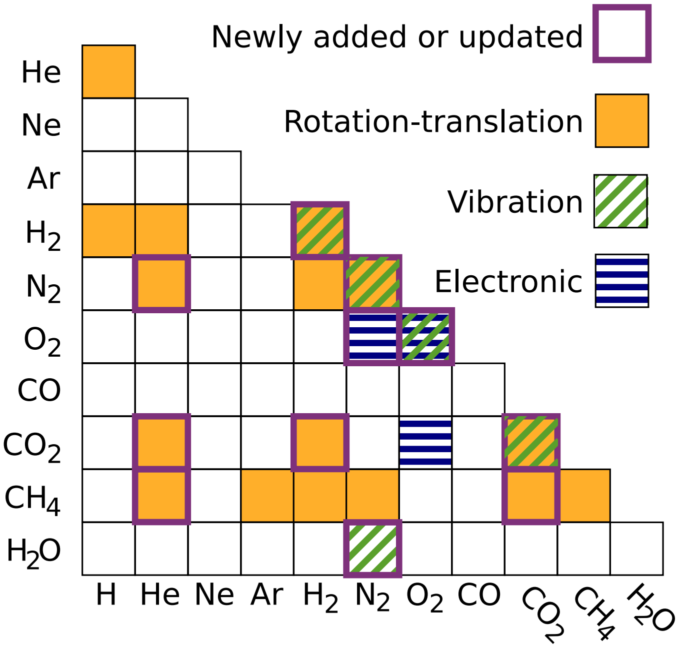
[1] Richard, et al., *J. Quant. Spectrosc. Rad. Transf.*, 113, 1276 (2012).



Newly added or updated □

Rotation-translation 🟧

Vibration ▨

Electronic ☰

	H	He	Ne	Ar	H_2	N_2	O_2	CO	CO_2	CH_4	H_2O
He	🟧										
Ne											
Ar											
H_2	🟧	🟧			□🟧▨						
N_2		□🟧			🟧	□🟧▨					
O_2						□☰	□☰▨				
CO											
CO_2		□🟧			□🟧		☰		□🟧▨		
CH_4		□🟧		🟧	🟧	🟧			□🟧	🟧	
H_2O						□▨					

Figure 2

“Main” and “Supplementary” folders. The main folder contains recommended sets of collision-induced absorptions whereas the supplementary folder contains two types of data. One type is the data alternative to that in the main folder. This is especially characteristic for the O_2-X complexes (see the corresponding section for details). In these cases “altern” is added to the filenames. Another type of data in the “Supplementary” folder is when the data is provided however one has to be cautious as we expect uncertainties in presented parameters are likely to be large. A wish list to eliminate remaining deficiencies or lack of data from the astrophysics perspective is also presented.

P-16. Measurement of Temperature-Dependent N_2-N_2 Collision-Induced Absorption and H_2-Broadening of Cold and Hot CH_4

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We report final results from two laboratory measurements on N_2-N_2 collision-induced absorption (CIA) in the far-infrared and H_2-broadened CH_4 in the near infrared region, respectively.

(1) The N_2-N_2 CIA coefficients have been measured in the 30–300 cm^{-1} at temperatures from 78 to 130 K by using a Fourier transform spectrometer (Bruker IFS-125HR) at Jet Propulsion Laboratory, configured with a coolable multipass White-type gas cell that was designed and built at the University of British Columbia. The cell mirror separation is 1 m and measurements were conducted using an absorption pathlength of 52 m. The temperature was monitored by four platinum resistors mounted on the exterior of the cell, and the cell pressure was measured by a capacitance pressure transducer. The N_2 and He gases used had stated purities of 99.999%, and gas pressures were between 0.6 and 2.5 atmospheres. Our measurements show stronger absorption than is predicted by the models. For the temperatures 78.3, 89.3, 109.6, and 129.0 K, the measurements at the peak exceed the Borysow models by 19, 14, 10, and 8%, respectively. The measurements at 129.0 K exceed those previously reported by Dagg et al.[1] at 126 K by 9% with stated measurement errors of ±10%. Further details on these measurements, and their deviations from models with respect to temperature, will be discussed in the presentation.

(2) In support of the Jovian and exoplanet atmospheric remote sensing in the near infrared, H_2-broadened CH_4 spectra were obtained at a broad temperature range between 80 and 370 K. For this, three custom-built gas absorption cells (two cold and one hot) were used, which are configured to a high-resolution Fourier transform spectrometer at JPL. The spectra have been analyzed with a non-linear multispectrum curve fitting

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[1] I. R. Dagg, et al., *Canadian J. Phys.*, 64, 1467-1474 (1986).

program package (along with recently developed graphical-user-interface version), which adopted speed-dependent non-Voigt line shape model with the line mixing effects taken into account. The retrieval results for the line parameters from the manifolds from P(4) through R(6), including H_2-broadened half widths, frequency shifts, and their temperature dependences will be presented and compared with published values currently available only at room temperature for the methane Octad band.

P-17. Water Vapor Line-Broadening Coefficients for Molecules in the HITRAN Database

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The new edition of the HITRAN database (HITRAN2016[1]) has substantially increased the potential for the database to model radiative processes in the terrestrial and planetary atmospheres. Water vapor in our atmosphere is highly variable which causes water to represent a potentially significant cross-sensitivity source. With that the water vapor is a very efficient broadener in comparison to nitrogen and oxygen and make an observable impact on the retrievals especially in the tropics. Interestingly, the atmospheres of rocky planets that may have suffered giant impacts are expected to have "steamy" atmospheres. For purpose of characterizing and reducing uncertainties in modeling the spectra of atmospheres with significant amounts of water vapor, the line-shape parameters for the line-broadening coefficients and the temperature dependence exponents for molecules of terrestrial interest broadened by water vapor were investigated through both experimental and theoretical studies. As a first step, oxygen broadened by water vapor was successfully investigated. A clear rotational dependence of H_2O broadening coefficients of O_2 lines was observed and then fitted by an empirical law[2,3,4,5]. Empirical Law used for fitting:

$$\gamma_{H2O} = A + \frac{B}{1 + c_1 x + c_2 x^2 + c_3 x^4} \tag{1}$$

We also performed similar investigation[6] for water vapor broadening coefficients of CO_2, CH_4, CO, NH_3, N_2O, OCS, CH_3CN and H_2CO lines. As a final step, a complete data set for all these broadening parameters due to pressure of water vapor will be implemented into the HITRAN database and will improve the accuracy of remote-sensing experiments in the future.

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[1] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[2] T. Delahaye, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 184, 316-321 (2016).

[3] B. J. Drouin, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 133, 190-198 (2014).

[4] G. Fanjoux, et al., *J. Chem. Phys.*, 101, 1061-1071 (1994).

[5] M. A. Koshelev, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 154, 24-27 (2015).

[6] Supported by NASA AURA and PDART program grants NNX14AI55G and NNX16AG51G.

P-18. H_2, He and CO_2 Line-Broadening Coefficients for Molecules in the HITRAN Database. Part II: CO_2, N_2O, H_2CO, HCN, H_2S, OH

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The new HITRAN database edition[1] features broadening and shift parameters due to the planetary perturbing gases such as H_2, He and CO_2 which had been added into the database for the first time, see Wilzewski et al.[2] In order to increase the potential for the database to model the spectra of atmospheres dominated by gases different from nitrogen and oxygen, especially in planets beyond the earth, including Venus[3] and Mars[4], and gas giants, the previous work accomplished by Wilzewski et al., which includes molecules for SO_2, NH_3, HF, HCl, OCS and C_2H_2, needed to be expanded further.

In this work[5], the line-shape parameters for the line-broadening coefficients and the temperature dependence exponents for molecules including CO_2, N_2O, OH, H_2CO, HCN and H_2S broadened by H_2, He, and CO_2 have been assembled from available peer-reviewed experimental and theoretical results. A set of semi-empirical models was developed based on the collected data, and then has been populated into the database so that every HITRAN line of the studied molecules has its corresponding parameters as well as its uncertainties and source information.

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[1] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[2] J. S. Wilzewski, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 168, 193-206 (2016).

[3] Exploration of Venus [Special Issue], *Planet. Space Sci.*, 113-114, 1-394 (2015).

[4] Dynamic Mars [Special Issue], *Icarus*, 251, 1-338 (2015).

[5] Supported by NASA PDART program grant NNX16AG51G

P-19. Applications of Complex Refractive Index Data for Aerosols: Case Studies for Stratospheric Aerosols

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Aerosol radiative forcing depends on the location of the aerosol, its composition, and its physical details (particularly its size). Depending on these details, the aerosol may introduce a positive or negative net perturbation to the balance between these incoming and outgoing radiative flows. A quantitative understanding of aerosol perturbations to the climate radiative balance requires a detailed understanding of the processes that govern radiative transfer in the atmosphere. These processes rest on fundamental optical properties, such as the complex refractive index, of the condensed phase materials that constitute aerosols. In situ measurements of stratospheric aerosols have revealed that aerosol composition includes significant contributions more species that just sulfuric acid and water. Organic carbon and mineral inclusions are two frequently found species. To understand the radiative perturbations attributable to aerosol containing these components requires wavelength-dependent data for aerosol optical depth, scattering efficiency, and scattering phase. Radiative forcing is primarily due to scattering and absorption of infrared radiation. Infrared absorption leads, in the stratosphere, to temperature increases, which both influence stratospheric dynamics and chemistry, and can cause additional modulations of radiative forcing itself. For multi-component species, particle morphology also must be known. Case studies will be presented for different assumptions about composition, season, and location for multi-component stratospheric aerosols. Using refractive index data from the HITRAN database, radiative forcing and radiatively-induced temperature changes will be calculated. Uncertainties due to shortcomings in the current state of knowledge about aerosol composition and morphology will be highlighted. These uncertainties are relevant not only to radiative forcing estimates, but also to measurement results from both remote sensing approaches and from in situ measurements that utilize optical measurement techniques.

P-20. HITRAN Application Programming Interface and Efficient Spectroscopic Tools (HAPIEST)

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Current high-resolution spectroscopic data have become more and more complex and extensive. In order to make a connection between the spectroscopic data in different formats and spectra observed in different applications, one needs a reliable and flexible tool, which is easy to use and deploy.

The HITRAN Application Programing Interface and Efficient Spectroscopic Tools (HAPIEST) is the joint project which started in the fall of 2017 as a collaboration between the HITRAN team and the State University of New York (Oswego). The purpose of HAPIEST is to simplify experiences using the HITRAN Application Programing Interface[1,2] (HAPI) to work efficiently with the HITRAN database HITRAN[3]. HAPIEST provides cross-platform graphical interactive tools giving access to the basic features of HAPI such as data fetching and selection, as well as generating and plotting of the spectral functions (absorption coefficients, transmittance, absorption, and radiance spectra).

HAPIEST provides interactive access to most of the controls which are involved in the spectral filtering and simulation, and is distributed both as binary and source code. The recent version of the source code can be found on Github[4]. The HAPI library, on which the HAPIEST is based, is a free open-source Python module (library) which provides a set of tools for working with the structured spectroscopic data from different sources. The principal aim of HAPI is facilitating physically-sound interpretation of observations and more realistic models for a wide variety of applications such as astrophysics, planetary science, climate simulations, remote sensing, theoretical spectroscopy, and data mining. Having such a tool is important in particular to prevent possible errors in radiative transfer calculations caused by misuse of spectroscopic tools and databases. The description of the first version of HAPI and its features can be found in the dedicated paper[1] and on the official web page[2].

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[1] R. V. Kochanov, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 177, 1530 (2016).

[2] http://hitran.org/hapi

[3] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2017).

[4] https://github.com/hitranonline/hapiest

P-21. Expanding Bytran Capabilities with Hardware Sensors and Device Interconnect

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We describe new functionality implemented in the bytran software[1] since its original release including the upcoming update to version 1.3. The new features include the support of external and built in hardware sensors for semi-empirical modeling and bytran communication capability for remote control and data retrieval.

The hardware sensor support was introduced to provide an option to acquire empirical data from ambient meteorological sensors (temperature, humidity and total pressure) for calculations as an alternative to manual entry. The sensors supported by bytran 1.2 include the external SensorTag module over Bluetooth[2], and the currently limited use of the built in cell phone sensors[3]. The Raspberry Pi's Sense Hat[4] support is planned for version 1.3.

To enable simplified integration of bytran into existing hardware systems without the need in source code modifications the capability to control bytran remotely was implemented in version 1.3. Such remote operation may be carried out over the Internet (with Bluetooth and the Serial Port support planned) using the newly introduced bytran communication protocol[5] and a variety of computer languages and programming environments. In particular, bytran execution over the Internet is based on the WebSockets protocol. WebSockets communication may be carried out using a wide array of programming languages including HTML5 and JavaScript from within a web browser. As such simple web-based applications may be developed to remotely control and retrieve calculation results from bytran[6] running on dedicated hardware such as a cell phone.

The above new features were meant to improve usability and make it relatively easy to integrate bytran into existing hardware systems. The near-term future plans for further bytran improvements include code optimizations to increase speed and the implementation of the Hartmann-Tran lineshape profile.

Recently Qt bindings with the Python language have gained attention due to the increased popularity of the Python language. Libraries implementing such capability include PySide and the PyQt. There has been recent work to extend their support to the Android and iOS operating systems. Originally developed as a separate branch

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[1] D. Pliutau, K. Roslyakov, *Earth Sci. Inform.*, 10, 395 (2017).

[2] http://www.ti.com/sensortag

[3] http://doc.qt.io/qt-5/compatmap.html

[4] https://www.raspberrypi.org/products/sense-hat/

[5] http://www.bytran.org/protocol.htm

[6] http://www.bytran.org/websockets.htm

PySide is to become included[7] into the main Qt development environment at the end of 2018. This opens a future possibility of creating a hybrid application by combining the bytran's cross platform Qt interface with the HAPI's Python computational code to function under mobile and desktop environments.

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[7] http://blog.qt.io/blog/2018/02/22/qt-roadmap-2018/

P-22. The Smithsonian PLanetary ATmosphere interface to VLIDORT (SPLAT-VLIDORT)

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The explosion of Earth atmosphere observations from space was a challenge for accurate and fast radiative transfer model (RTM) calculations. Over the years we have developed the capabilities needed for real time processing of large datastreams. The use of such Earth-centric RTMs in planetary applications has been limited by their complexity. In light of this we have developed a flexible and user-friendly FORTRAN interface to VLIDORT, a discrete ordinate RTM for polarized light.

The Smithsonian PLanetary ATmosphere interface to VLIDORT (SPLAT-VLIDORT) retains features for Earth simulations whilst being capable of simulating more general situations. Features include:

- User-specified major atmospheric constituent inputs needed for Rayleigh scattering.
- User-specified gas absorption inputs, including allowances for collision induced absorption and HITRAN-based pressure-temperature lookup tables.
- A flexible cloud/particle scattering interface, with additional tools for customizable scattering properties.
- Anisotropic treatment of surface reflectance, based on semiempirical BRDF kernels.

We will illustrate some of the capabilities of the new interface with simulations of Earth radiance observations from the upcoming TEMPO geostationary satellite mission.

P-23. New Method to Establish Frequency Calibration of FTS with Multireflection Cells

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In laboratory FT spectroscopy in the infrared region, instrumental line shape (ILS) determination and the associated frequency calibration is necessary for accurate measurements. For high pressure measurements, both can be obtained from a previous measurement of a calibration gas at low pressure, preferably under otherwise similar conditions. However, especially in combination with a multireflection cell, a subsequent change in pressure causes an alteration in the adjustment of multireflection cell due to mechanical deformations and change of refractive index. The beam path and profile are thus shifted, which especially comes into effect for high absorption paths. An unavoidable correction of the adjustment then usually causes a deviation from the original ILS and thus from frequency calibration. ILS contributions are distributed over the infrared beam in the spectrometer optics and therefore the adjustment can influence the ILS. Especially the detector and detector window exhibit a strong angular dependence of reflectivity, thus influencing the ILS.

The known method of using a small cell with a calibration gas in series with the multireflection cell fails when narrow band filters are applied for obtaining good signal to noise ratios and there is no calibration gas available with strong lines in the spectral region of interest.

Here, a method is presented by which the re-adjustment of the instrument can be performed in a way to restore the previous ILS and frequency calibration for large absorption paths and pressure changes of about 1 bar. Explained is the detailed restoring procedure as well as exemplary results using a multireflection cell of 0.8 m base length set to an absorption path of more than 100 m, where a secondary reference cell was used to validate the method.

P-24. Ammonia Spectra in the Cryogenically Cooled Herriott Cell

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A 7 m path long cryogenically cooled Herriott cell was used to probe ammonia absorption in two spectral regions. In the mid-infrared the Vertical External Cavity Surface Emitting Laser[1] was used in the 4275–4355 cm^{-1} range and couple of New Focus external cavity diodes lasers covered the 6500–6800 cm^{-1} range in the near infrared[2,3,4]. The absorption spectra were recorded for the two main isotopologues in the temperature range from 122 to 300 K with the temperature accuracy of ±0.15 K. Most recently, investigation of the deuterated isotopologues began with the observation of the ND_2H and NH_2D species.

Besides the spectroscopic description of ammonia isotopologue and comparison with the most recent studies (e.g., Al Derzi, et al.[5], Yurchenko[6], Barton, et al.[7]), the topic of the presented contribution is to discuss the improved method for measurements of lower state energies of transitions with datasets from independent spectra.

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[1] P. Čermák, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 137, 13–22 (2014).

[2] P. Cacciani, et al., *J. Quant. Spectrosc. Radiat. Transf* 113, 1084–1091 (2012).

[3] P. Cacciani, et al., *Mol. Phys.*, 112, 2476–2485 (2014).

[4] J. El Romh, et al., *J. Mol. Spectrosc.*, 326 122-129 (2016).

[5] A. Al Derzi, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 161, 117–130 (2015).

[6] S. Yurchenko, *J. Quant. Spectrosc. Radiat. Transf.*, 152, 28–36 (2015).

[7] E. Barton, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 189, 60–65 (2017).

P-25. The Effect of Diffusivity Factor Approximation on the Representation of Spectral Outgoing Longwave Radiation

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The infrared outgoing longwave radiation (OLR) flux is calculated through an angular integration of directionally dependent radiances over zenith angle. To reduce computational labor in the process, a common technique is to use the radiance intensity obtained along a specific zenith angle to approximate the isotropic radiance, known as Diffusivity-factor approximation[1]. The choice of diffusivity factor has been intensively discussed over the past half-century, and it is mathematically determined to be $e^{1/2} = 1.6487213$ using a one-node Gaussian quadrature method (1GQ)[2].

However, the proposed diffusivity factor may not properly represent spectral OLR for several reasons. First, the 1GQ method residual is dependent on optical depth, leading to error with opposite signs between window bands and absorption bands. Second, the optical transmission path is simplified to straight-line-of-sight, such that earth geometry and path refraction are not considered. The curvature of path thus increases the limb-view optical depth of the lower atmosphere, adding further uncertainties. Third, as weighting function varies greatly across the spectral, the summation of OLR contributed from each vertical level is hard to be represented by one diffusivity factor.

This study investigates into the spectral error of DF approximation with path curvature and tests the feasibility of using band-dependent diffusivity factor. It is found that the DF approximation overestimates window band OLR by 3% while underestimates CO_2 and O_3 contribution by around 1.5%, resulting from a combination of path curvature effect and GQ method residual. In the window band, the contribution from both surface and atmosphere are important, in which case, the choice of diffusivity factor is not only dependent on optical depth. Therefore, we suggest a latitudinal and seasonal dependent diffusivity factor for the 11 bands over infrared spectral.

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[1] W. M. Elsasser (1942). *Heat Transfer by Infrared Radiation in the Atmosphere.* Harvard Meteorological Studies, Vol. 6, Harvard University Press, 107.

[2] J. Li, *J. Atmospheric Sci.*, 57, 753-765 (2000).

P-26. A Scaled Linear Retrieval Technique for Tropospheric Pollutants

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Fast retrieval methods for the detection of tropospheric trace gases from hyperspectral nadir sounding satellite observations (e.g., IASI) often provide unreliable total column measurements. Alternatively, more accurate iterative retrieval methods require large processing times, making them inadequate for near-real time monitoring. We present a scaled linear retrieval method that aims to provide a better estimate for the total column of tropospheric trace gases (e.g., NH_3, SO_2), while remaining fast to compute and appropriate for near-real time retrievals. The performance of this method is compared to current retrieval methods for NH_3.

P-27. High-Spin Electronic States of Molecular Oxygen

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As a by-product of an ongoing rather comprehensive study of the electronic structure of the lowest valence and Rydberg states of O_2, chiefly singlets and triples, in this contribution we focus on high-spin electronic states, namely, quintets and septets. Although these latter states may be thought of as of pure academic interest, the current calculations show interesting features of their potential energy curves (PECs) which have not been studied and are actually unknown for most diatomics made up of first-row atoms (plus hydrogen and helium). Experimentally, there is essentially no information whatsoever, aside from some indirect evidence of the possible involvement of high-spin species in the spectroscopy or photodissociation processes. Theoretically, there are a few studies, but they are usually issued from early and modest calculations, so the accuracy is not good enough.

We report in this contribution an insight into the quintet and septet electronic states of molecular oxygen. Their PECs display a rich and complex structure, and interactions among states which could not be anticipated. We report PECs of valence, Rydberg and ion-pair quintet states as well as of various Rydberg septet states. Most PECs are repulsive, as expected, yet, a few of the high-spin states are bound. Excitation energies are tabulated for all states. Spectroscopic constants are given for the bound states. A case is also presented of a bound sextet state of O_2^+, along with potential curves of several sextet repulsive states of the cation.

SESSION III: Exoplanets and Stars

III-1. Characterization of Exoplanet Atmospheres via Molecular and Atomic Spectroscopy

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Obtaining information about the chemical composition and the physical conditions in the atmospheres of exoplanets is crucial for improving our understanding of the physical processes that govern planet formation and evolution. The main observing techniques for atmospheric characterization are transmission and emission/reflection spectroscopy. Although major advances have been made over the past decade, there are still many challenges associated with the interpretation of exoplanet spectra, which is why we need to keep searching for new probes of exoplanet atmospheres that are complementary to the currently existing diagnostics. In the context of molecular spectroscopy, I will discuss one such method, based on the detection of spectral signatures of Raman scattering on atmospheric molecules at short visible wavelengths. High-resolution spectra of atomic lines, on the other hand, can give us valuable insights into the structure and properties of the upper layers of exoplanetary atmospheres, i.e. thermospheres and exospheres. I will present recent results on using the helium triplet line at 1083 nm as a new window into the extended exoplanet atmospheres, which can be used to improve our understanding of atmospheric escape and mass loss in close-in exoplanets.

III-2. The Calculation of Atomic and Molecular Opacities for Astrophysical Applications

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In order to properly model and study the emergent spectra of a variety of astronomical objects it is necessary to adequately model the opacity of their atmospheres. The objects of interest to our group span a range of temperatures from very cold solar system objects to the lower temperature limits of stellar atmospheres. There is also a large range in pressures from fractions of a millibar to hundreds of bars. An added complication is that, unlike the typical stellar atmosphere that is predominantly neutral or ionized hydrogen and helium, these objects have atmospheres that are mainly molecular hydrogen and helium. In some cases involving hypothetical rocky planets that have suffered giant impacts there may be high concentrations of water (steam) or other volatiles. This creates problems for properly defining the line broadening parameters and even the line shape itself.

Another major challenge can be the very large size of certain molecular data sets that contain tens of billions of lines. As astronomical objects may span a large range of temperatures in a given atmosphere there is a real challenge at high temperatures when you have to do line-by-line calculations with such large data sets. I will review how our own group currently handles these problems and how others have suggested alternative approaches. I will emphasize the need for better data and discuss some of the many challenges including getting line widths for species and broadeners that are not usually studied either in the lab or through computational simulations. I will also point out what will be needed as the resolution of astronomical observations improves in the future.

III-3. Planetary Spectrum Generator: An Accurate Online Radiative Transfer Suite for Atmospheres, Comets, Small Bodies and Exoplanets

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We have developed an online radiative-transfer suite[1] applicable to a broad range of planetary objects (e.g., planets, moons, comets, asteroids, TNOs, KBOs, exoplanets). The Planetary Spectrum Generator (PSG) can synthesize planetary spectra (atmospheres and surfaces) for a broad range of wavelengths (UV/Vis/near-IR/IR/far-IR/THz/sub-mm/Radio) from any observatory (e.g., JWST, ALMA, Keck, SOFIA), any orbiter (e.g., ExoMars, Juno), or any lander (e.g., MSL). This is achieved by combining several state-of-the-art radiative transfer models, spectroscopic databases and planetary databases (i.e., climatological and orbital). PSG has a 3D (three-dimensional) orbital calculator for most bodies in the solar system, and all confirmed exoplanets, while the radiative-transfer models can ingest billions of spectral signatures for hundreds of species from several spectroscopic repositories. It integrates the latest radiative-transfer and scattering methods in order to compute high resolution spectra via line-by-line calculations, and utilizes the efficient correlated-k method at moderate resolutions, while for computing cometary spectra, PSG handles non-LTE and LTE excitation processes. PSG includes a realistic noise calculator that integrates several telescope / instrument configurations (e.g., interferometry, coronagraphs) and detector technologies (e.g., CCD, heterodyne detectors, bolometers). Such an integration of advanced spectroscopic methods into an online tool can greatly serve the planetary community, ultimately enabling the retrieval of planetary parameters from remote sensing data, efficient mission planning strategies, interpretation of current and future planetary data, calibration of spectroscopic data, and development of new instrument/spacecraft concepts.

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[1] https://psg.gsfc.nasa.gov

III-4. Fast Spectral Synthesis for a New Generation of Solar and Stellar Brightness Variability Models

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Regular space-borne observations revealed that solar brightness varies on timescale from minutes to decades. Concurrently, photometric measurements of Sun-like stars uncovered similar variations. Whereas the Sun's variability has impact on the Earth's atmosphere and in turn on the climate, stellar brightness variations are a limiting factor for the detectability and habitability of exoplanets. The brightness variations of the Sun and Sun-like stars are fully controlled by the Fraunhofer lines present all over their spectra. In particular, Fraunhofer lines define the amplitude of the stellar brightness variability on timescales greater than a day and in case of the Sun even the phase of the solar brightness variability over the 11-year magnetic activity cycle. Molecular lines play a special role is stellar brightness variations due to their strong sensitivity to temperature chances. For example, the maximum of the absolute spectral brightness variability of the Sun is associated with the CN violet system.

Recently a new generation of models for solar and stellar variability, based on the 3D magnetohydrodynamics simulations of the stellar atmospheres and state-of-the art radiative transfer approaches, has appeared. A huge amount of Fraunhofer lines makes calculations with such models extremely time consuming. Building on the well-known approach of the opacity distribution functions (ODFs) we have developed a more efficient method to account for the Fraunhofer lines in the radiative transfer calculations: the optimised opacity distribution functions (OODFs). Such a method takes the current models of solar and stellar brightness variations to a new level and makes it possible to investigate a whole range of a new phenomena. The applications of our method is not limited to modelling brightness variations and we believe it to be useful for a broad community of researches working on the radiative transfer in stellar, solar, and planetary atmospheres. To obtain comprehensive OODFs an accurate treatment of the underlying atomic and molecular lines is needed. We plan to incorporate the latest and most complete linelists (and especially utilise HITRAN for the molecular linelists) before making our routines and data publicly available.

SESSION IV: Theoretical Linelists for Exoplanets

IV-1. The ExoMol Project: Progress and Perspectives

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The ExoMol project aims to provide molecular line lists for exoplanets and other atmosphere with a particular emphasis on those atmospheres which are significantly hotter than the Earth's[1]. ExoMol has now computed line lists for about 40 molecules including, in most cases, isotopologues. These are available at www.exomol.com. Key new line lists include ones for H_3^+ [2], NO [3], C_2H_4 [4] and a significantly improved one for hot water[5], as well as for a range closed and open shell diatomic molecules.

The ExoMol database underwent a major reformat and upgrade in 2016 [6]; it now provides information on a variety of topics including, of course, line lists, cross sections (generated from the same line lists), lifetimes and Landé g-factors. Our new flexible code ExoCross can rapidly generate cross sections even from huge line lists. ExoCross[7] also allows facile conversion between ExoMol and HITRAN formats.

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[1] J. Tennyson, S. N. Yurchenko, *Mon. Not. R. Astr. Soc.*, 425, 21 (2012).

[2] I. I. Mizus, et al., *Mon. Not. R. Astr. Soc.*, 468 1717 (2017).

[3] A. Wong, et al., *Mon. Not. R. Astr. Soc.*, 472, 882 (2017).

[4] B. P. Mant, A. Yachmenev, J. Tennyson, S. N. Yurchenko, *Mon. Not. R. Astr. Soc.*, in press.

[5] O. L. Polyansky, et al., *Mon. Not. R. Astr. Soc.*, in press.

[6] J. Tennyson, S. N. Yurchenko, ExoMol Team, *J. Mol. Spectrosc.*, 372, 73 (2016).

[7] S. N. Yurchenko, A. F. Al-Refaie, J. Tennyson, *Astron. Astrophys.*, in press.

IV-2. TheoReTs – *Ab Initio* Based Information System For Astrophysical Applications: Line Lists, Cross-Sections And Validation Versus Observed Spectra

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TheoReTS[1,2,3] – is an information system for theoretical spectra based on variational predictions from molecular potential energy and dipole moment surfaces for various molecular species of interest for planetology and astrophysical applications jointly developed by Reims and Tomsk teams[4].

The current TheoReTS implementation contains information on four-to-six atomic molecules, including phosphine, methane, ethylene, silane, methyl-fluoride, tetrafluoromethane, germane and their isotopic species $^{13}CH_4$, $^{12}CH_3D$, $^{12}CH_2D_2$, $^{12}CD_4$, $^{12}C_2H_4$. An extension to deuterated isotopologues PH_2D, PHD_2, $C_2H_2D_2$, $^{12}C^{13}CH_2D_2$, C_2H_3D[5] and to NF_3, H_2CO is in progress. Predicted hot ethylene data up to 700 K and of methane line lists up to T = 3000 K[6,7] are included. The information system provide associated software for spectra simulation including absorption coefficient, absorption and emission cross-sections, transmittance and radiance. The simulations allow Lorentz, Gauss and Voight line shapes. Rectangular, triangular, Lorentzian, Gaussian, sinc and sinc squared apparatus function can be used with user-defined specifications for broadening parameters and spectral resolution. All information is organized as a relational database with the user-friendly graphical interface.

The validations of recent *ab initio* predictions for rotationally resolved spectra of

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[1] M. Rey, Y. Babikov, A. Nikitin, V. Tyuterev, *J. Mol. Spectrosc.*, 327, 138 (2016).

[2] http://theorets.univ-reims.fr

[3] http://theorets.tsu.ru

[4] Supports from ANR e-PYTHEAS and Mendeleev funding Tomsk State University grant are acknowledged.

[5] D. Viglaska, et al., Poster at this Workshop : HITRAN (2018) – see page 27.

[6] M. Rey et al., *Aston. Astrophys.*, 594, A47 (2016).

[7] M. Rey et al., *Astrophys. J.*, 847, AA8909 (2017).

related molecules with respect to high-resolution experimental data[8,9,10], low resolution records (PNNL experimental library), Titan atmospheric observations[11] and comparisons with HITRAN and GEISA databases will be discussed.

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[8] A. Wong, et al., Poster at this Workshop : HITRAN (2018) – see page 28.

[9] R. Georges, et al., private communication.

[10] M. Rey, et al., *Phys. Chem. Chem. Phys.*, 18, 176 (2016).

[11] M. Rey, et al., *Icarus* 303, 114 (2018).

IV-3. The Spectroscopy of C_3: New Challenges and New Physics

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We discuss first principles calculations of electronic transitions in C_3. The challenges are the need for explicitly including diagonal corrections to the Born-Oppenheimer approximation, the need to generate diabatic states to untangle avoided crossings, and the limitations of currently available electronic structure methods. In the process of overcoming these challenges, we have encountered a very unusual breakdown of the Born-Oppenheimer approximation.

IV-4. Molecular Simulations for the Spectroscopic Detection of Biosignature Gases and Other Volatiles

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Unambiguously identifying molecules in spectra is of fundamental importance for a variety of scientific and industrial uses; a compelling modern focus is the spectroscopic detection of volatiles in exoplanet atmospheres, and the assessment of habitability and inhabitability of these planets. Analyses of observational spectra require information about the spectrum of each of its putative components. However, spectral data currently only exist for a few hundred molecules and only of fraction of those have complete spectra (e.g., H_2O, NH_3). Consequently, molecular detections in exoplanet atmospheres are vulnerable to false positives, false negatives and miss-assignments. There is a key need for spectral data for a broad range of molecules.

Using a combination of experimental measurements, organic chemistry, and quantum mechanics, ATMOS (Approximate Theoretical MOlecular Spectra) is a programme that:

(a) Provides approximate spectral data (band centres and relative intensities) for thousands of molecules in seconds.

(b) Assesses hundreds of molecules simultaneously, highlighting patterns and any distinguishing features. Traditional methods for obtaining spectra are extremely costly and time-consuming (i.e., months/years per molecule); ATMOS will inform prioritization protocols for future high accuracy studies.

(c) Demonstrates that, at low resolution, individual spectral features could belong to a large number of molecules. Molecular detections in spectra are often made by assigning one, or a few, spectral features to a given molecule. ATMOS can highlight ambiguities in such molecular detections and also direct observations towards spectral regions that reduce the degeneracy in molecular identification.

IV-5. Sub-percent accuracy for the intensities of top five HITRAN molecules

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Recent progress on the high accuracy intensity calculations of H_2O, CO_2, ozone, CO and N_2O is described. The need for high accuracy line intensities for these molecules for the modelling atmospheres of the Earth and exoplanets is well-established. The three major factors for accurate intensity calculations are the nuclear motion program, accurately fitted potential energy surface (PES) to the experimental rovibrational energy levels and high accuracy *ab initio* dipole moment surface (DMS). The details of use of these three factors for the sub-percently accurate line intensities of the molecules, listed as the first five most important molecules in HITRAN database, will be given. In particular, the results of our calculations on the IR lines of H_2O[1,2] and CO_2[3,4,5,6] have been incorporated into the HITRAN2016 database. The new results on water IR and optical-UV region will be presented as well as O_3[7], CO and N_2O line intensities calculations.

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[1] L. Lodi, J. Tennyson and O. L. Polyansky, *J. Chem. Phys.*, 135, 034113 (2011).

[2] M. Birk, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 88-102 (2017).

[3] O. L. Polyansky, et al., *Phys. Rev. Lett.*, 114, 243001 (2015).

[4] E. Zak, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 177, 31-42 (2017).

[5] E. Zak, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 189, 267-280 (2017).

[6] E. Zak, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 265-281 (2017).

[7] O. L. Polyansky, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 210, 127-135 (2018).

SESSION V: Spectroscopy of the Terrestrial Atmosphere

V-1. Atmospheric Spectroscopy at the Smithsonian Astrophysical Observatory: From Mount Sinai to Geostationary Orbit and Beyond

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I will address the solar and atmospheric measurements at SAO beginning with its establishment in 1890, through the establishment of an observatory on Mount Saint Katherine (Zebel Gebir), a spur of Mount Sinai, in 1933, with the assistance of Archimandrate Joakim and the monks of the Monastery of Saint Katherine on Mount Sinai, to more recent balloon, aircraft, ground, and satellite-based measurements of the physics and chemistry of the stratospheric ozone layer, climate-altering greenhouse gases, and atmospheric pollution. There will be a brief excursion into the atmospheric spectroscopy of exoplanets.

V-2. Spectroscopy for Remote Sensing of Tropospheric Composition: Perspectives from the Aura-TES and OCO-2 Teams

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(on behalf of the TES and OCO-2 ABSCO and algorithm teams)

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The accuracy of remotely-sensed quantities depends directly on the accuracy of the spectroscopic input to the forward model used in the retrievals (line shape, line parameters and continuum). Here, we provide perspectives on spectroscopy-related needs and challenges for two NASA satellite missions that measure trace gases in the troposphere: the Aura Tropospheric Emission Spectrometer (TES) and the Orbiting Carbon Observatory reflight (OCO-2).

TES, a Fourier transform spectrometer measuring thermal infrared radiances at high spectral resolution (0.1 cm^{-1} apodized), was launched on the Aura satellite in July 2004 and decommissioned in January 2018. The TES radiances have been used to retrieve estimates of temperature, H_2O and a range of different tropospheric trace gases, including O_3, CO, HDO, CH_4, CO_2, NH_3, CH_3OH, HCOOH, OCS and PAN. Molecular absorption coefficients are pre-calculated and stored in look-up tables for use within the TES retrieval algorithm. We discuss the spectroscopic input currently used in the calculation of these tables and highlight outstanding sources of systematic error affecting the analysis of the radiance measurements from TES and other thermal-infrared spaceborne spectrometers.

The Orbiting Carbon Observatory (OCO-2), launched in July 2014, is a grating spectrometer measuring in the 0.76 micron O_2 A-band and the 1.61 and 2.06 micron CO_2 bands. The OCO-2 radiances are analyzed to yield estimates of the CO_2 dry air mole fraction, X_{CO2}. Look-up tables of molecular absorption coefficients are also utilized within the OCO-2 algorithm. Retrievals of well-mixed greenhouse gases such as CO_2 place particularly stringent demands on the accuracy of the forward model, since the variations of these gases in the atmosphere are small compared to the background. The goal for OCO-2 is to obtain X_{CO2} with accuracy of 0.25% (1 ppm out of the 400 ppm background), in order to understand carbon sources and sinks on regional scales over the globe. To accomplish this goal, it will be necessary to simulate spectral radiances to an accuracy of around 0.1%. This places particularly stringent demands on the spectroscopic input to the retrieval algorithm. We discuss recent developments and ongoing efforts to reduce systematic errors associated with spectroscopy in the OCO-2 forward model. We show results of validation of the current version of absorption coefficients using ground-based atmospheric measurements from the Total Carbon Column Observing Network (TCCON) as well as spectral residuals from OCO-2 retrievals. We highlight remaining challenges in the OCO-2 bands, including accuracy of absolute intensity measurements for CO_2, the representation of line mixing (LM) for CO_2 and O_2, collision induced absorption (CIA) for O_2 and temperature dependence of LM and CIA. Finally, we point to new, high signal to noise laboratory measurements (Cavity Ring Down Spectroscopy from NIST and Photoacoustic Spectroscopy from the California Institute of Technology) and associated multispectrum fitting analysis underway to address these challenges.

V-3. Re-evaluating the Use of O_2 $a^1\Delta_g$ Band in Spaceborne Remote Sensing of Greenhouse Gases

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[c]*Environment and Climate Change Canada, Toronto, Ontario, Canada*

[d]*School of Engineering and Applied Sciences and Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA, USA*

Although the O_2 $a^1\Delta_g$ band has long been used in ground-based greenhouse gas remote sensing to constrain the light path, it is challenging for nadir spaceborne sensors due to strong mesosphere/stratosphere airglow. Spectroscopic simulations using upper state populations successfully reconstruct the airglow spectra with excellent agreement with SCIAMACHY limb observations (residual root-mean-square $< 0.7\%$). The accurate knowledge of airglow spectrum enables retrieval of $O_2(a^1\Delta_g)$ number density, volume emission rate, and temperature. For nadir spaceborne observations, the $a^1\Delta_g$ airglow will lead to a negative bias of $\sim 10\%$ to O_2 column, if not considered. However, when properly included, the airglow spectral feature can be adequately separated from O_2 absorption (mean bias $< 0.1\%$) at the spectral resolution of modern spaceborne spectrometers.

V-4. Satellite Remote Sensing of the Atmosphere: Past (MIPAS) and Future (FORUM) Challenges

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Satellite remote sensing techniques are widely used to measure the chemical and physical state of the Earth atmosphere and of the atmospheres of other planets. These techniques rely on the measurement of the atmospheric spectrum, in a variety of spectral ranges. In particular, remote sensing measurements of the atmospheric and Earth emitted radiation are performed in the Infrared and Far-Infrared spectral regions, where most of the black body emission at their temperatures is located. To extract information from these measurements on the atmospheric state, very accurate knowledge of the spectroscopy of the atmospheric major and minor gases is required. The retrieval of the vertical profiles of temperature and atmospheric constituents is usually performed by fitting to the observations a full-physics model taking into account emission and absorption of all molecules. As a consequence the quality of the retrievals is directly linked to the availability and accuracy of the spectroscopic parameters.

MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) was a Fourier transform spectrometer designed for the measurement of the Earth atmospheric limb emission in the thermal infrared (TIR) spectral range (685–2410 cm^{-1}). It flew onboard the polar orbiting ENVISAT satellite for approximately 10 years, from June 2002 to April 2012, performing measurements during both day and night with relatively high spectral resolution (0.025 cm^{-1} in the first part of the mission and 0.0625 cm^{-1} in the second part). MIPAS/ENVISAT measurements represent a unique database for the study of the vertical distribution and time variation of the atmospheric composition on a global scale with data on more than 20 minor atmospheric constituents. On top of that, the high resolution of MIPAS measurements has provided a unique benchmark for the accuracy of current spectroscopic data.

FORUM (Far-infrared-Outgoing-Radiation Understanding and Monitoring) is a new sounder selected by ESA for the phase A studies for the selection of the future Earth Explorer 9 mission. It has been designed to measure the complete spectrum of the Earth outgoing long wave radiation from space including the FIR (Far InfraRed) spectral region for the first time ever. The instrument will measure the top of the atmosphere radiation in the FIR TIR spectral regions (from 100 to 1600 cm^{-1}) with a spectral resolution of 0.3 cm^{-1}. On top of that, FORUM will provide information on the vertical distribution of water vapour, temperature and other minor constituents. The exploitation of the FIR spectral range (100–667 cm^{-1}) poses new requirements for the knowledge of the spectroscopy in this so-far unexploited spectral region.

Here we will report some of the results of spectroscopic studies driven by MIPAS and the results of the sensitivity studies to spectroscopic data performed for the FORUM proposal.

V-5. Spectroscopy Issues for the Atmospheric Chemistry Experiment

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The Atmospheric Chemistry Experiment is a satellite-based mission for remote sensing of the the Earth's atmosphere. The primary instrument on board is a high resolution (0.02 cm^{-1}) Fourier transform spectrometer (FTS) operating in the infrared (750–4400 cm^{-1}). It has been collecting solar occultations measurements for more than 14 years. A mission overview will be presented, along with a description of the new processing version for the FTS (version 4.0) that is currently underway. The spectroscopic line list employed for version 4.0 processing is based primarily on HITRAN 2016. Spectroscopic issues encountered with this line list will be discussed.

V-6. CO_2 Spectroscopy and Forward Modelling Accuracy in the Thermal Band: An Assessment Study with IASI Spectral Observations

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The Infrared Atmospheric Sounder Interferometer (IASI) has been demonstrated to be both radiometrically and spectrally stable[1] and therefore its observations are particularly suited for assessment studies of spectroscopy and forward modeling accuracy. Towards this objective we have used a suitable set of IASI soundings recorded over the GRUAN (Global climate observing system (GCOS) Reference Upper-Air Network) validation station of Manus (Papua New Guinea, 2.06°S, 147.42°E, 6 m asl). The set of observations has been recorded from January to June 2014, until the station has been active. Night-time, clear sky, sea surface soundings have been considered in order to avoid non-LTE problems in the CO_2 ν_3 band. IASI soundings have been complemented with Temperature and H_2O mixing ratio profiles, which have been continued to the upper stratosphere through the use of time-space collocated ECMWF analysis. Care has been particularly taken to collocate IASI soundings with radiosonde observations and ECMWF analysis. Because Manus is close to the equator, we could exploit the satellite crossing time close to 12 UTC, which also coincides with one of the canonical hours of radiosonde launch and ECMWF analysis. In this way, collocation is performed better than 30 min in time and better 50 km in space.

Spectroscopy and forward modelling accuracy have been assessed by computing spectral residuals (Observations-Calculations). Calculations have been performed with our forward/inverse model, φ-IASI, which uses the whole IASI spectral coverage and retrieve all surface and atmospheric parameters, which IASI is sensitive to[2].

Our forward model σ-IASI is a monochromatic radiative transfer code, which uses a look table of monochromatic optical-depth computed by LBLRTM (Line-by-Line Radiative Transfer Model). For the present analysis the look-up table is derived from LBLRTM model version 12.4, which in turn is based on the Atmospheric Environmental Research or AER v_3.4 line parameter database with the continuum absorption MT_CKD 2.5.7.[3]

The analysis shows that the CO_2 ν_2 spectral region, which is probing the troposphere, yields a spectral residual within the IASI noise already with the temperature and water vapor radiosonde observations. Upon retrieval, we have a complete consistency, within

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[1] C. Camy-Peyret et al., *J. Quant. Spectrosc. Radiat. Transf.*, 201, 197-208 (2017).

[2] G. Liuzzi et al., *J. Quant. Spectrosc. Radiat. Transf.*, 182, 128-157 (2016).

[3] e.g., see http://rtweb.aer.com/lblrtm_frame.html

IASI noise, both in CO_2 ν_2 and N_2O/CO_2 ν_3 spectral regions. We will show that initial discrepancy in the CO_2 ν_2 spectral region, which is probing the stratosphere, is due to ECMWF temperature profile inadequacy in the upper stratosphere. Furthermore, we show that the CO_2 ν_2 and N_2O/CO_2 ν_3 spectral regions show a consistent behavior for channels, which are probing the troposphere.

Based on these findings, we have used IASI observations to derive CO_2 column amount for a 4-years long record (2014–2018) of IASI soundings close to the Mauna Loa validation station (Hawaii). The analysis shows that CO_2 column amount can be derived solely from the data, without the use of heavy constraints, which is the common practice with CO_2 retrieval from Space. The results confirm that state of art CO_2 spectroscopy and related improvement in Line Mixing[4] are accurate enough to yield CO_2 retrievals with unprecedented accuracy.

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[4] J. M. Hartmann et al., *J. Quant. Spectrosc. Radiat. Transf.*, 213, 178-227 (2018).

V-7. Evaluating Different HITRAN Databases Using AIRS and CrIS

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Satellite hyperspectral infrared sounders for Numerical Weather Prediction have been operational for almost 20 years. This era began with NASA Atmospheric Infrared Sounder (AIRS) in May 2002 in a 1:30 orbit, followed by EUMETSAT's IASI in 2007 in the 9:30 orbit. The AIRS record is now supplemented with the Cross Track Infrared Sounder (CrIS) on the Suomi platform (October 2011) and more recently on the NOAA-20 (November 2017). Our group has provided fast radiative transfer algorithms (RTAs) for all of these instruments to NASA (AIRS, CrIS) and NOAA (CrIS, IASI) for operational 1D-var retrievals. We have used our own line-by-line algorithms, fast monochromatic algorithms (kCARTA), and AER's LBLRTM to generate the inputs for these satellite RTAs. These satellite sounders are particularly sensitive to spectral line shape models (line-mixing), continuum models (H_2O), and non-LTE emission. We provide an overview of the status of these fast models, particularly in the context of present uncertainties in their accuracy using various validation approaches.

V-8. Low-Temperature, High-Precision Measurements of the O_2 A-Band

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The remote sensing of atmospheric species such as CO_2 typically requires the determination of column-integrated airmass from co-located observations of O_2 A-band transmission spectra. To avoid airmass-dependent biases in the retrieved concentration of the target species, the most accurate and precise measurements require predictive models of transmitted solar irradiance in the O_2 A-band region. Previous studies have shown that these models must account for the temperature- and pressure-dependence of advanced line shapes, line mixing (LM), and collisional induced absorption (CIA). Although a recently published self-consistent model of the O_2 A-Band accounted for these effects, it was compromised by the lack of high-resolution, low-temperature measurements in the R-branch region. In this work, we report recent measurements of the entire O_2 A-band which were made with a variable-temperature cavity ring-down spectroscopy system. Spectra were acquired over the temperature, pressure and O_2 molar fraction ranges of (220 K – 290 K), (6.6 kPa – 133 kPa) and (0.2 – 15%), respectively. The low-range molar fraction data provides information on the temperature dependence of advanced line shape parameters such as speed dependence, while higher mole fraction data corresponding to optically thick samples can be analyzed to yield the LM and CIA model parameters. This work is expected to reduce uncertainty in predicted temperature- and pressure-dependent O_2 A-band absorption cross sections for use in retrieval algorithms such as those used by the Orbiting-Carbon Observatory-2 Mission.

V-9. Multispectrum Analysis of the Oxygen A-Band

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[c]*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, USA*

Composition measurements from remote sensing platforms require knowledge of air mass to better than the desired precision of the composition. Oxygen spectra allow determination of air mass since the mixing ratio of oxygen is fixed. The OCO-2 mission is currently retrieving carbon dioxide concentration using the oxygen A-band for air mass normalization. The 0.25% accuracy desired for the carbon dioxide concentration has pushed the state-of-the-art for oxygen spectroscopy. To produce atmospheric pressure A-band cross-sections with this accuracy requires a sophisticated line-shape model (Rautian or Speed-Dependent) with line mixing (LM) and collision induced absorption (CIA). Models of each of these phenomena exist, but an integrated self-consistent model must be developed to ensure accuracy.

This presentation will describe the ongoing effort to parameterize these phenomena on a representative data set created from complementary experimental techniques. The techniques include Fourier transform spectroscopy (FTS), photoacoustic spectroscopy (PAS) and cavity ring-down spectroscopy (CRDS). CRDS data allow long-pathlength measurements with absolute intensities, providing lineshape information as well as LM and CIA, however the subtleties of the lineshape are diminished in the saturated line-centers. Conversely, the short paths and large dynamic range of the PAS data allow the full lineshape to be discerned, but with an arbitrary intensity axis. Finally, the FTS data provides intermediate paths and consistency across a broad pressure range. These spectra are all modeled with the Labfit software using first the spectral line database HITRAN, and then model values are adjusted and fitted for better agreement with the data.

SESSION VI: Laboratory Measurements

VI-1. Recent Progress in the Infrared Spectroscopy of Ozone

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The recent and unpublished results on the ozone spectra analyses will be reported here. All the spectra have been recorded on the Fourier Transform Spectrometer of GSMA (Reims) in Infrared with resolution of 0.002 cm^{-1}.

(1.) $^{16}O_3$

The spectra of main isotopologue of ozone were analyzed in 5 and 10 microns regions, 3735 transitions were assigned belonging to the dyad $\{(100)/(001)\}$ up to $J = 81$ and 6336 transitions to the triad $\{(200)/(101)/(002)\}$. The observed data were modelled with *rms* deviations of 0.12×10^{-3} cm^{-1}; the strongest lines are obtained with the precision better than 4×10^{-5} cm^{-1}.

In the whole spectral domain, the transitions affected by local resonances are replaced by observed ones through changes of energy levels. The intensities of the ν_1 and ν_3 bands were revisited, the resulting calculated line list shows good agreement with recent *ab initio* calculation[1]. In the 5 microns range, the problem of inconsistencies among different microwindows[2] is now resolved.

(2.) $^{16}O^{16}O^{18}O$

Spectra of quasi pure ozone generated from various $^{18}O_2$–$^{16}O_2$ mixtures have allowed observing and assigning 15 bands of the most abundant isotopic species $^{16}O^{16}O^{18}O$ in the atmosphere in the 950–3900 cm^{-1} spectral range. These bands were fully analyzed, leading to the assignment of a total of 9976 transitions, corresponding to 7030 energy levels. The analyses were performed using appropriate effective Hamiltonian and effective dipole transition moment operators with the help of theoretical predictions on the band centres, rotational constants and part of coupling parameters[3,4].

(3.) ^{17}O enriched isotopic species

The FTS spectra of ozone generated from mixtures of ^{17}O, ^{16}O and ^{18}O oxygen atoms were recorded in the 5 and 10 microns ranges. This mixture leads to the formation of

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[1] Vl. G. Tyuterev, R. Kochanov, S. Tashkun, *J. Chem. Phys.*, 146, 064307 (2017).

[2] C. Janssen, et al. *J. Mol. Spectrosc.*, 326, 48-59 (2016).

[3] Vl. G. Tyuterev, R. Kochanov, S. Tashkun, *Proceedings of XVII International Symposium HighRus-2012*, 6 (2012).

[4] Vl. G. Tyuterev, et al., *J. Chem. Phys.*, 139, 134307 (2013).

18 isotopic species, mainly enriched by ^{17}O. In addition to already analyzed species[5,6,7], we were able to assign and analyze ν_3 and $\nu_1+\nu_3$ bands of four isotopologues of ozone: ^{17}O^{17}O^{18}O, ^{17}O^{18}O^{17}O, ^{17}O^{17}O^{16}O and ^{17}O^{16}O^{17}O. The retrieved parameters are in good agreement with theoretical predictions[3,4]. All these new results will be included in the S&MPO information system[5].

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[5] S. N. Mikhailenko, Y. L. Babikov, Vl. G. Tyuterev, A. Barbe, *Comput. Technol.*, 7, 64-70 (2002).

[6] http://smpo.iao.ru

[7] http://smpo.univ-reims.fr

VI-2. New Spectroscopic Data for Tropomi/S5P in the 2.3 μm region for CH_4 and H_2O and a New UV Database for Ozone

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The ESA project "SEOM-Improved Atmospheric Spectroscopy Databases (IAS)" will improve the spectroscopic database for retrieval of the data products CO, CH_4, O_3 and SO_2 column amounts measured by the TROPOMI instrument (TROPOspheric Monitoring Instrument) aboard the Sentinel-5 Precursor. The project was launched in February 2014 with 3 years duration extended to 2018.

New spectroscopic data have been obtained for CO, CH_4 and H_2O in the 2.3 μm region. Measurements were mainly taken with a high resolution Fourier Transform spectrometer combined with a coolable multi reflection cell. Cavity ring down measurements served for validation. While water analysis with multispectrum fitting turned out to be straight forward the analysis of methane turned out to be very complicated and time consuming. The input database HITRAN2012 was found to be not suitable as initial guess and a theoretical database provided by V. Tyuterev and A. Nikitin was used instead. Still about 2900 misplaced/new lines (1300 lines removed) were found which required pure methane measurements at low and ambient temperature in order to fit the lower state energy of the unassigned lines. In order to fit the spectrum down to the noise level speed dependence, Rosenkranz line mixing and temperature dependence of line mixing had to be considered. The data quality of the new database was validated by solar occultation measurements where residuals showed solar lines only, but no spectroscopic database error. Furthermore, atmospheric CH_4 profiles in agreement with models could be obtained using the new spectroscopic data, for the first time. The significant impact of the new spectroscopic data with respect to HITRAN2012 for CH_4 and CO columns for TROPOMI observations was derived by retrieval simulations.

New UV measurements for a new temperature dependent absorption cross section database for O_3 have been carried out. Large effort has been taken to ensure a good baseline and to obtain highly accurate number densities in the cell. The new database shows good agreement (better than 1%) with other databases for the 253 nm mercury line, but 1–2% lower values above 330 nm in the region relevant for atmospheric remote sensing. Together with our new MIR results[1] these results also could close the 4% gap between UV and infrared atmospheric observations.

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[1] see presentation "New Absolute and Relative Line Intensities of Ozone Fundamentals – A Step Towards the End of the Ozone UV/MIR Dilemma" on page 78.

VI-3. New Absolute and Relative Line Intensities of Ozone Fundamentals – A Step Towards the End of the Ozone UV/MIR Dilemma

G. Wagner,[a] **M. Birk**,[a] **J.-M. Flaud**,[b] **A. Barbe**,[c] **M.-R. de Backer**,[c]
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[c] *Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France*

New ozone mid infrared measurements in the frame of an ESA project (SEOM-IAS) have been carried out at DLR and Reims. These measurements were combined with previous measurements taken in 1998 and published in 2002[1]. The analysis was performed with a multispectrum fitting approach. It turned out that the treatment of the instrumental lineshape has a large influence on the line intensities in case of nearly Doppler-broadened measurements. Furthermore, it was found that without considering speed dependence the line intensities for measurements even in the 1 mbar range were too small by about 1%. Self speed dependence was expressed in terms of a polynomial versus the Lorentzian self broadening.

Alternatively, the approach by H. Tran et al.[2] was used to calculate the speed dependence from the temperature exponent of the Lorentzian self broadening, which was available since one of the measurements was recorded at 233 K. The absolute and relative line intensities were found to be significantly different from HITRAN, where the relative line intensities have remained unchanged for 26 years. The new line intensities in the ν_3 region, which is most relevant for atmospheric applications, were larger by 2% for weak and up to 4% for strong lines.

It should be noted that atmospheric ozone retrievals pointed out a discrepancy of about 4% when ozone was retrieved from infrared and UV measurements. An increase of MIR ozone line intensities would partly close this gap. A new quantum mechanical treatment of the new data will also be presented. The results given are based on DLR measurements alone. A spectrum from a Reims measurement was used for validation.

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[1] G. Wagner, M. Birk, F. Schreier, J.-M. Flaud, *J. Geophys. Res.*, 107, 4626 (2002).

[2] H. Tran, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 111, 2012-2020 (2010).

VI-4. Measurements of Ozone Line Intensities at 5 and 10 μm

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[c]*Sorbonne Université, CNRS, Institut des NanoSciences de Paris, INSP, 75005 Paris, France*

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In the present study, high resolved (resolution of 0.002 cm^{-1}) Fourier transform ozone spectra have been recorded both around 5 μm and 10 μm from the same sample of gas. For that a "H" shape cell has been used (see Figure 3) in order to have a 20 cm absorption path length for the region at 5 μm and a 5 cm absorption path length at 10 μm.

The rapid scan interferometer Bruker IFS 125 from QualAir platform allowed us to record alternatively the 5 μm and 10 μm spectral regions every hour. Interferograms were recorded for one hour at 5 μm, then 2 hours were dedicated for the 10 μm region. This scheme was repeated 4 times during approximately 12 hours. Consequently, almost simultaneous recording of the 2 spectral regions (with same amount of ozone) have been

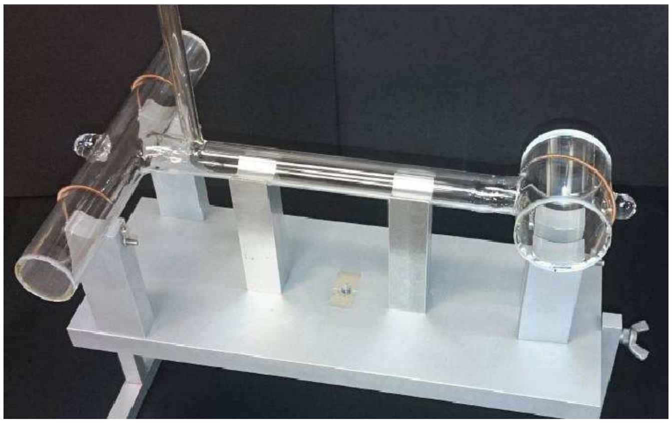

Figure 3

performed allowing to get rid of relative errors mainly due to the quantity of ozone in the cell. In order to reach quantitative measurements, the pressure of ozone in the cell has been continuously monitored by UV measurements at 252.65 nm. Cross sections from the literature have been averaged in order to deduce accurate pressure of ozone in the cell.

The analysis of the 2 spectral regions was carefully performed on isolated transitions, taking into account small apparatus function effects as the finite size of the beam in the interferometer. Effect of such correction is in this case in the order of 1% which is not negligible for ozone line intensity measurements. A multispectrum fitting procedure was used to retrieve final set of line parameters based on the analysis of 6 spectra recorded with different pressures of ozone. Around 800 and 600 transitions have been analyzed in the 10 μm and 5 μm regions respectively. Comparison of line intensities from this work and those from literature and databases will be presented.

VI-5. Comb-Assisted CRDS of Water Vapor: From Extensive Spectral Coverage to Doppler-Free Saturation Dips

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In the last years, we have combined our high sensitivity cavity ring down spectrometers to an auto-referenced frequency comb to address different aspects of water vapour spectroscopy:

(i) The room temperature absorption spectrum of water vapour highly enriched in ^{17}O was studied by comb assisted-cavity ring down spectroscopy (CA-CRDS) between 1.50 μm and 1.26 μm (6667-7921 cm^{-1})[1,2]. As a consequence of the high sensitivity of

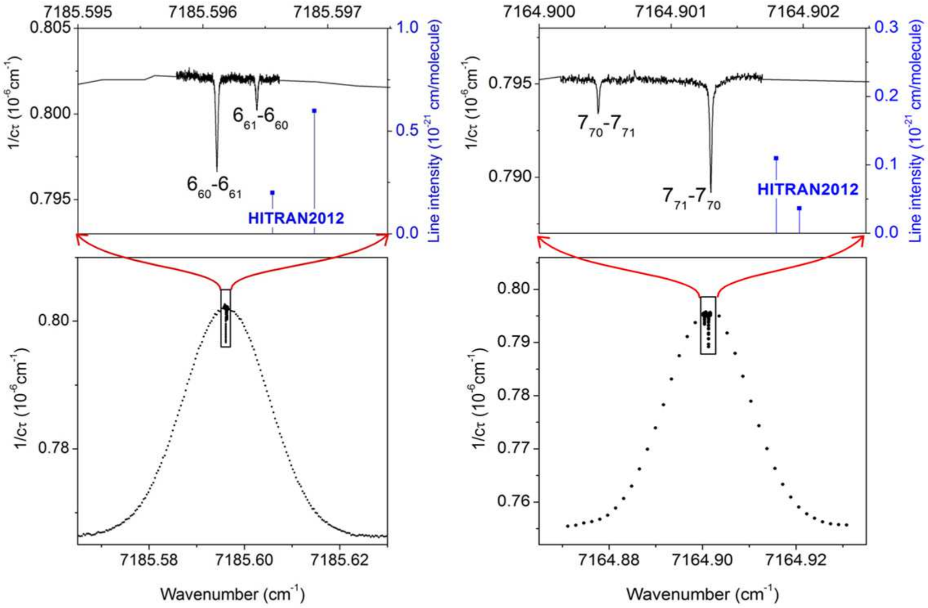

Figure 4: Absorption line and Lamb dips for the $J_{J0} \leftarrow J_{J1}$ and $J_{J1} \leftarrow J_{J0}$ doublets of $H_2{}^{16}O$ (J= 6, 7). On the lower panels, individual measurements points are showed to illustrate the higher resolution to sampling the dips range.

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[1] S. N. Mikhailenko et al., *J. Quant. Spectrosc. Radiat. Transf.*, 206, 163-171 (2018).

[2] D. Mondelain et al., *J. Quant. Spectrosc. Radiat. Transf.*, 20, 206-212 (2017).

the recordings (noise equivalent absorption, $\alpha_{min} \approx 10^{-10}$ cm^{-1}), a series of spectra could be recorded at very low pressure (less than 0.1 Torr) allowing for accurate determination of line centres and the spectral resolution of highly blended multiplets. Overall, the experimental list includes more than 14,000 water lines which were assigned to six isotopologues ($H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, $HD^{16}O$, $HD^{17}O$ and $HD^{18}O$). Their intensities span seven orders of magnitude from 10^{-28} to 10^{-21} cm molecule^{-1} at 296 K. The center values of non blended lines are reported with an accuracy better than 3 MHz (10^{-4} cm^{-1}) which represents an improvement compared to previous determinations (in particular for the main isotopologue, $H_2{}^{16}O$). The comparison to the water vapor line list provided by the 2016 version of the HITRAN database reveals a number of issues.

(*ii*) Doppler-free saturated-absorption Lamb dips were measured at sub-Pa pressures on rovibrational lines of $H_2{}^{16}O$ near 7180 cm^{-1}, using optical feedback frequency stabilized cavity ring-down spectroscopy[3]. By referencing the laser source to the optical frequency comb, transition frequencies were determined down to 100 Hz precision and kHz accuracy. The developed setup allows resolving highly K-type blended doublets ($J_{J0} \leftarrow J_{J1}$ and $J_{J1} \leftarrow J_{J0}$) separated by about 10 MHz (Figure 4), providing valuable tests for spectroscopic databases and recent variational calculations.

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[3] S. Kassi et al., *J. Chem. Phys.*, 148, 054201 (2018).

VI-6. Investigation of the ν_8 and ν_{21} Bands of Propane at 11.5 and 10.9 μm: Evidence of Large Amplitude Tunnelling Effects

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We present the first investigation of the ν_8 B-type band (870.3 cm^{-1}) of propane ($CH_3CH_2CH_3$) together with an extended analysis of the neighbouring ν_{21} A-type band[1] (921.4 cm^{-1}). For both bands the rotational energy levels in the 8^1 and 21^1 upper states are split because of interactions with the internal rotations of the methyl groups, leading to the identification of AA, EE, AE and EA torsional components. An effective "vibration - torsion - rotation" Hamiltonian model was built in the G_{36} symmetry group, which shows that these torsional splittings are due to the existence of anharmonic and Coriolis resonances, coupling the 8^1 and 21^1 rotational levels to nearby highly excited levels of the two internal rotations of the methyl groups. Accordingly, a code computing the line intensities was developed to allow unambiguous torsional component identifications. The line assignments were performed using a high resolution (0.0015 cm^{-1}) IR spectrum of propane, recorded at 142 K using the French SOLEIL synchrotron facility coupled to a Bruker IFS125HR Fourier transform spectrometer. A list of individuals line positions and intensities to be used for the detection of propane in the Earth and outer planets atmospheres was produced and compared with the existing pseudolines[2] or cross sections[3].

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[1] A. Perrin, et al., *J. Mol. Spectrosc.*, 315, 55 (2015).

[2] K. Sung, G. C. Toon, A. W. Mantz, M. A. H. Smith, *Icarus*, 226, 1499 (2013).

[3] A. Wong, R. J. Hargreaves, B. Billinghurst, P. F.Bernath, *J. Quant. Spectrosc. Radiat. Transf.*, 198, 141 (2017).

VI-7. Quantitative Infrared Spectroscopy of Halogenated Species for Atmospheric Remote Sensing

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Fluorine- and chlorine-containing molecules in the atmosphere are very strong greenhouse gases, meaning that even small amounts of these gases contribute significantly to the radiative forcing of climate. In addition, a number of these molecules, such as chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs), are harmful to the Earth's ozone layer and for this reason their use is regulated by the 1987 Montreal Protocol. The recent Kigali Amendment has added hydrofluorocarbons (HFCs) to the list of controlled substances, coming into effect on 1 January 2019. HFCs, which do not deplete stratospheric ozone, were introduced as refrigerant replacements for CFCs and HCFCs. They are potent greenhouse gases, with global-warming potentials many times greater than carbon dioxide, and are increasing in the atmosphere at a very fast rate.

A number of satellite instruments can monitor these species, in particular the Atmospheric Chemistry Experiment Fourier transform spectrometer (ACE-FTS), a high resolution (0.02 cm^{-1}) instrument covering the 750–4400 cm^{-1} spectral region in solar occultation mode. With long atmospheric pathlengths ($\sim$300 km) and the sun as a radiation source, the ACE-FTS measures the vertical profiles of more molecules in the atmosphere than any other satellite instrument.

Quantification of the atmospheric abundances of these halogenated species requires accurate quantitative infrared spectroscopy. HITRAN contains absorption cross section datasets for a number of these species, but many of them have minor deficiencies that introduce systematic errors into satellite retrievals. This talk will focus on new and improved laboratory spectroscopic measurements for a number of these important halogenated species.

VI-8. Precise Line Positions from Laser-Locked Cavity Ring-Down Spectroscopy

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S.-M. Hu[a]

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Line positions are the most frequently referenced information from the spectral database. However, the accuracy of most absorption line positions in the near infrared is limited to 10^{-3}–10^{-4} cm^{-1} due to the broadening effects (Doppler and collision induced) and/or the weakness of the overtone transitions. Using the method of laser-locked cavity ring-down spectroscopy, where the laser frequency is tightly locked to the cavity and eventually locked with an optical frequency comb, we realized spectroscopy with ultra-high precision and high sensitivity as well. Taking advantages of the power enhancement by the cavity, we are able to record saturation spectra of molecular overtone transitions in the near infrared using continuous-wave diode lasers of milli-Watt power. As a demonstration, Lamb dips of ro-vibrational transitions of CO at 1.6 μm were recorded and their positions were determined with sub-kHz (10^{-8} cm^{-1}) accuracy[1]. Precise positions of water vapor[2] and acetylene[3] transitions near 0.8 μm were also determined with an accuracy of a few kilohertz (10^{-7} cm^{-1}). The accuracy of the line positions were also investigated by the analysis of ground state combination differences.

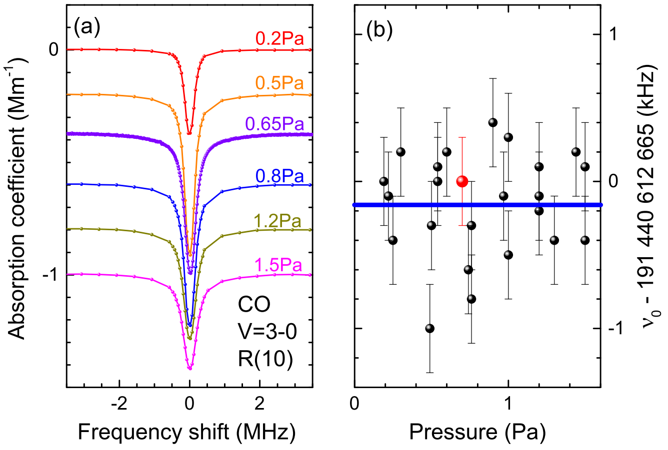

Figure 5: (a) Saturation spectra of the R(10) line in the (3-0) band of $^{12}C^{16}O$. (b) Line positions determined from spectra recorded with different sample pressures.

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[1] J. Wang, et al., *J. Chem. Phys.*, 147, 091103 (2017).

[2] J. Chen, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 205, 91 (2018).

[3] L.-G. Tao, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 210, 111 (2018).

VI-9. Molecular Line Intensities of Carbon Dioxide in the 1.6 μm Region Determined by Cavity Ringdown Spectroscopy

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Here we present some recent advances in frequency stabilized cavity ring-down spectroscopy (FS-CRDS) measurements of molecular line intensities of carbon dioxide in the (30012) ← (00001), the (30013) ← (00001) and (30014) ← (00001) bands. The FS-CRDS spectrometer used to carry out most of these measurements has been described extensively in previous work[1] and provides precise and accurate measurements of line shape parameters and intensities. We also measured the (30012) ← (00001) band with another spectrometer based on the frequency-agile rapid scanning (FARS) CRDS technique, also described previously[2]. This latter approach provides an independent measurement platform with dramatically higher acquisition rates, allowing for a more complete survey and assessment of our measurement uncertainty. All sample temperatures were near 296 K and were actively regulated at the tens of mK level. For each transition, spectra were acquired at four pressures, from 8.7 kPa to 20 kPa. We also used certified CO_2-in-air gaseous samples with SI-traceable mixing ratios nominally equal to 390 μmol/mol for the (30012) and (30013) CO_2 bands and 1% for the relatively weak (30014) band. All temperature, pressure and amount-of-substance measurements were SI-traceable. Ring-down spectra were acquired on samples in a flowing configuration at a nominal flow rate of 0.04 L/min to minimize wall effects and outgassing.

We compared the line intensities (based on fits of the Hartmann-Tran Profile to measured spectra) to those reported in several spectroscopic databases, including the *ab initio* calculations reported by Zak et al. (i.e., HITRAN 2016)[3]. The overall agreement between these results and the *ab initio* calculations of Zak et al. is excellent[3], although some individual transitions show deviations of up to 1%. Comparisons between measured and calculated intensities for the (30012) ← (00001) show average agreement and relative standard deviations at the 0.1% level. Preliminary measurements on the (30013) ← (00001), and the (30014) ← (00001) bands in this region also show good agreement with the *ab initio* calculations of Zak et al. for the (30013) ← (00001), but considerably poorer agreement for the (30014) ← (00001) band. No significant J-dependence up to J ~ 30–40 was observed for any of the three bands. We have

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[1] H. Lin, Z. D. Reed, V. T. Sironneau, J. T. Hodges, *J. Quant. Spectrosc. Radiat. Transf.*, 161, 11-20 (2015).

[2] G. W. Truong, et al., *Nat. Photonics*, 7, 532-534 (2013).

[3] E. J. Zak, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 189, 267-280 (2017).

previously reported agreement at the 0.3% level for the (30013) ← (00001) with *ab initio* calculations[4], and have recently demonstrated agreement at the 0.3% level for the (20012) ← (00001) band near 2 μm[5]. This work demonstrates significant improvement in the measurement of CO_2 line intensities in the 1.6 μm region, and provides independently determined uncertainties of theoretical line intensities. These results demonstrate the feasibility of achieving ‰-level relative uncertainties in *ab initio* calculations for global determinations of line intensities.

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[4] O. L. Polyansky, et al., *Phys. Rev. A*, 114, 243001 (2015).

[5] H. Yi, *J. Quant. Spectrosc. Radiat. Transf.*, 206, 367-377 (2018).

VI-10. Towards a Coherent Spectral Line Parameter Set for the Complete $2\nu_3$-Band of $^{14}N_2{}^{16}O$ Using High Resolution FTIR-Spectroscopy

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The Total Carbon Column Observing Network (TCCON) monitors the atmospheric abundance of the key greenhouse and ozone-depleting gas nitrous oxide (N_2O) using the $2\nu_3$-band of the most abundant isotopologue $^{14}N_2{}^{16}O$. For this purpose, spectral reference line parameters for this band are needed. The present reference data, however, show a lack with respect to a metrological determination and a detailed uncertainty analysis. Moreover, direct measurements in the $2\nu_3$-band are, partially, missing so that data from other spectral regions are used.

Within the scope of our recent high resolution (0.002 cm^{-1}) FTIR-spectroscopy studies[1,2,3] of N_2O, we determined a new and coherent spectral line parameter set for the R-branch of the $2\nu_3$-band. The individual spectra were measured at 296 K with special focus on metrological determination of the most relevant input parameters, i.e., pressure, temperature and absorption path length, and on a detailed uncertainty assessment. These input parameters are traceable to the SI[4,5]. Their respective uncertainties are determined according to the GUM[6,7,8]. The data set consists of line strengths and parameters for air- and self-induced broadening and shift. All parameters for the TCCON-window were experimentally determined in the $2\nu_3$-band with the same infrastructure including these lines which were missing so far.

In our present contribution, we extend our previous R-branch analysis of the measured high resolution FTIR-spectra also to the P-branch. Here, we report our results for line strengths and parameters for self-induced broadening and shift for rotational levels from $J = 1$ up to $J = 40$. For self-broadening and self-shift coefficients, for example, the uncertainties are reduced compared to literature data by a factor of up to 15 and 19, respectively. The future extension of our analysis to air broadening and air shift which is particularly important for the TCCON remote sensing network will be discussed.

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[1] V. Werwein, et al., *J. Mol. Spectrosc.*, 323, 28-42 (2016).

[2] V. Werwein, et al., *Appl. Opt.*, 56, E99-E105 (2017).

[3] V. Werwein, et al., *J. Mol. Spectrosc.*, in press.

[4] The International System of Units (SI), Bureau international des poids et mesures (BIPM), 2006.

[5] http://www.bipm.org/en/measurement-units

[6] Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement, International Organization for Standardization, 2008.

[7] http://www.iso.org/sites/JCGM/GUM-JCGM100.htm

[8] http://www.bipm.org/utils/common/documents/jcgm/JCGM_104_2009_E.pdf

The extension of our previous analysis was realized within the continuation of the EUMETRISPEC[9] project to establish a European spectroscopy infrastructure enabling measurements of spectral line parameters traceable to the SI.

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[9] www.eumetriscpec.org

SESSION VII: Lineshapes and Continua

VII-1. Line-Shape Problems in Modelling Laboratory and Atmospheric Spectra and Predictions of High-Order Line-Shape Parameters using Molecular Dynamics Simulations

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It is now well known that the widely-used Voigt profile does not well describe absorption line shapes of molecular gases. This is due to several collision effect which are neglected by the use of the Voigt profile such as the Dicke narrowing, the speed dependences of the collisional parameters, the collisional interferences between lines (line-mixing). Examples of the influence of these non-Voigt effects on the extraction of spectral line parameters from laboratory measured spectra as well as on atmospheric spectra analysis will be given. A short review on the recent theoretical approaches, models and results on the topic of isolated line shapes and of line-mixing will be presented. The last part of this presentation is devoted to the recent results obtained with the use of molecular dynamics simulations to predict line-shape parameters of refined line-shape models, with examples for CO, H_2O and O_2.

VII-2. First Comprehensive Dataset of Beyond-Voigt Line-Shape Parameters from *Ab Initio* Quantum Scattering Calculations for the HITRAN Database

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M. Konefał,[a,c,d] **S. Kassi,**[c,d] **A. Campargue,**[c,d] **Y. Tan,**[e,g] **J. Wang,**[e]
A.-W. Liu,[e] **S.-M. Hu,**[e] **K. Patkowski,**[f] **R. Ciuryło,**[a] **D. Lisak,**[a]
R. V. Kochanov,[g,h] **I. E. Gordon**[g]

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[c]*University of Grenoble Alpes, LIPhy, F-38000 Grenoble, France*

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[h]*Tomsk State University, Laboratory of Quantum Mechanics of Molecules and Radiative Processes, Tomsk, Russia*

Molecular collisions are manifested as a perturbation of the shapes of molecular optical resonances. Therefore, on one hand, the line-shape analysis of accurate molecular spectra constitutes an important tool for studying quantum scattering and testing *ab initio* molecular interactions. On the other hand, the collisional effects can deteriorate the accuracy of atmospheric measurements of the Earth and other planets, modify the opacity of the exoplanetary atmospheres as well as influence the accuracy in optical metrology based on molecular spectroscopy. Recently a new relational structure has been introduced to the most extensively-used line-by-line spectroscopic database HITRAN, enabling the collisional, beyond-Voigt line-shape effects to be represented. It is, however, extremely challenging to populate the entire database with purely experimental parameters for all the molecular transitions and thermodynamical conditions (all the bands, branches and temperature ranges).

We demonstrate a new methodology of generating a comprehensive dataset of the beyond-Voigt line-shape parameters from fully *ab initio* quantum-scattering calculations.

We also demonstrate first such a complete dataset for the helium-perturbed H_2 benchmark system. We provide the temperature dependences for the pressure broadening and shift parameters, as well as for the Dicke parameter using generalized spectroscopic cross sections resulting from quantum scattering calculations on accurate *ab initio* potential energy surfaces. The results are consistent with the recently adapted HITRAN parameterisation of the Hartman-Tran profile. The calculations and methodology are validated on the ultra-accurate experimental data recorded with cavity ring-down spectroscopy.

VII-3. Temperature Dependence of Half-Widths and Line Shifts for Molecular Transitions in The Microwave and Infrared Regions

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An expression was derived from an expansion of the optical cross-sections in powers of the radiator-perturber relative velocity, cut off at second order, that correctly models the temperature, T, dependence of the half-width, γ, over large temperature ranges and the T dependence of the line shift, δ, even for cases where the shift changes sign. Data were collected for more than 100 thousand transitions and the power law (PL) expression for γ and δ, when the shift doesnt change sign, were compared with the new double power law expression. Figure 6 shows data (symbols) and fits (solid lines) for the $2_{\,2\,0} \leftarrow 3_{\,1\,3}$ rotation band transition of H_2O in collision with H_2; left-hand upper

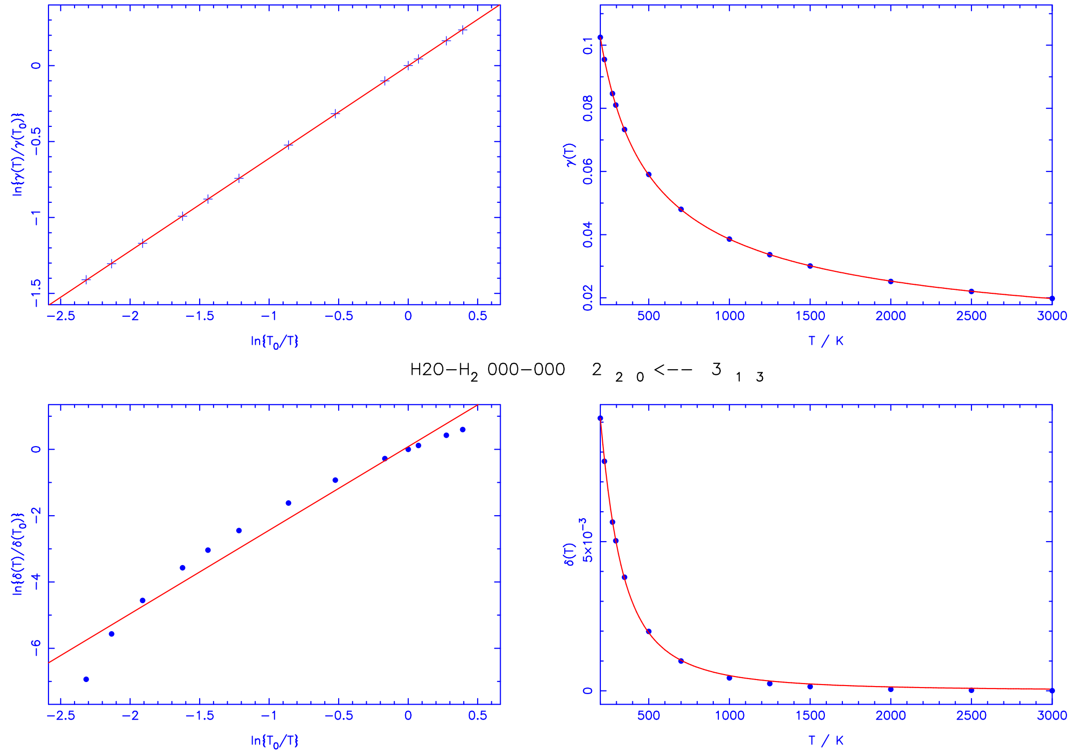

Figure 6

and lower panels are the PL fits for γ and δ, right-hand upper and lower panels are the DPL fits for γ and δ.

The DPL model gives much improved results for the half-widths and for line shifts, even those data that exhibit unusual structure, which the standard power law cannot model. For transitions where δ changes sign, the DPL model fits the data well. The DPL model for the T dependence of δ was compared with the linear model, which is currently used on the HITRAN database. In all cases, the DPL model gave much better results than the linear model, no matter what temperature range was studied. The new formalism allows a substantial reduction in the number of parameters needed to be stored in databases and the same expression can be utilized in radiative transfer and simulation codes for both the half-width and line shift.

VII-4. Line Shape Parameters for the 1←0 Bands of CO Isotopologues

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In 2012 we reported the results of studies of air- and self-broadened line shape parameters, including temperature dependences, in the 2←0 bands of $^{12}C^{16}O$, $^{13}C^{16}O$, and $^{12}C^{18}O$ based on analyses of high-resolution spectra recorded at temperatures from 150 to 298 K using Fourier transform spectrometers (FTS)[1,2]. We have now completed similar studies in the 1←0 bands of the same isotopologues using high-resolution spectra from two FTS systems: the Bruker IFS-125HR FTS at Jet Propulsion Laboratory (JPL) and the McMath-Pierce FTS at the National Solar Observatory on Kitt Peak, AZ. The JPL spectra were recorded with ^{13}C- or ^{18}O-enriched CO samples at temperatures from 149 K to 299 K, while the Kitt Peak spectra were recorded with a CO sample of natural isotopic abundance at temperatures between 79 and 296 K. Selected groups of 20 (for $^{12}C^{18}O$) or 21 (for $^{13}C^{16}O$) spectra from both FTS systems were analyzed by nonlinear least-squares multispectrum fitting to determine air-broadened line shape parameters, including temperature dependences and line mixing for the fundamental bands of these two isotopologues[3,4]. The multispectrum fitting algorithm was also applied to a group of 38 Kitt Peak spectra to determine line parameters including self- and air-broadening coefficients, pressure-induced shifts, and line-mixing parameters, including temperature dependences for $^{12}C^{16}O$ [5]. The results for the 1←0 bands will be compared with previous published measurements and calculations and with the current HITRAN[6] values.

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[1] V. Malathy Devi, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 113, 10131033 (2012).

[2] V. Malathy Devi, et al., *J. Molec. Spectrosc.*, 276, 3348 (2012).

[3] V. Malathy Devi, et al., *J. Quant. Spectrosc. Radiat. Transf.*, (2018) submitted.

[4] V. Malathy Devi, et al., International Symposium on Molecular Spectroscopy, Champaign-Urbana, IL, June 18-22, FF01 (2018).

[5] A. Predoi-Cross, et al., International Conference on Spectral Line Shapes, Dublin, Ireland, June 17-22 (2018).

[6] I. E. Gordon, et al., *J. Quant. Spectrosc. Radiat. Transf.*, 203, 3-69 (2016).

VII-5. Recent Enhancements to the MT_CKD Continuum: Part I

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D. D. Turner,[b] **S. Paine**,[c] **L. Palchetti**,[b] **G. Bianchini**,[d] **J. Delamere**,[e]
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[f] *Jet Propulsion Laboratory NASA, California Institute of Technology, Pasadena, CA, USA*

Various recent upgrades to the MT_CKD continuum will be presented. The enhancements that will be presented were derived from a number of different sources, including improvements to the far-IR/sub-millimeter/microwave (derived from ground-based measurements), and near-IR (lab measurements). Part II follows on page 98.

VII-6. Recent Enhancements to the MT_CKD Continuum: Part II

M. J. Alvarado,[a] **E. J. Mlawer,**[a] **K. E. Cady-Pereira,**[a] **R. Pernak,**[a]
D. D. Turner,[b] **S. Paine,**[c] **L. Palchetti,**[b] **G. Bianchini,**[d] **J. Delamere,**[e]
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A recent upgrade to the MT_CKD continuum in the mid-IR, based on lab, satellite, and ground-based measurements will be presented. This talk will start off where the previous MT_CKD talk ends. Part I precedes on page 97.

VII-7. Influence of Humidity on Absorption by N_2 and CO_2 Near 4 μm: Calculations, Comparisons with Measurements and Atmospheric Consequences

J.-M. Hartmann,[a] **H. Tran**,[a] **R. Armante**,[a] **C. Boulet**,[b] **G. C. Toon**[c]

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Molecular Dynamics Simulations (MDS) based on the use of the equations of classical mechanics and input intermolecular potentials are used for predictions of the time evolutions of the positions and orientations of ensembles of N_2-H_2O and CO_2-H_2O gas molecules[1]. From this knowledge, the interaction-induced dipole in N_2-H_2O pairs is determined at all times based on the long range induction mechanisms associated with the polarizabilities and electric multipoles of the molecules. The time auto-correlation function (ACF) of this dipole then yields the absorption spectrum, through Laplace-Fourier transform. For CO_2-H_2O pairs, the dipole moment (of CO_2) is obtained from the CO_2 axis orientations and the Laplace-Fourier transform of its ACF provides the spectrum. The results of such computations, in which no parameter was adjusted, are compared with measurements for N_2-H_2O[2] and CO_2-H_2O[3] absorptions near 4 μm. Equivalent previously made comparisons between experimental results and those of similar MDS computations for pure N_2[4] and pure CO_2[5] are also presented.

These comparisons show the quality of the theoretical calculations. Indeed, the latter predict both the magnitude and shape of the absorption spectra as well as the large differences between the effects of N_2-N_2 and N_2-H_2O collisions and those of CO_2-CO_2 and CO_2-H_2O interactions. This demonstrates the interest of the classical approach, in particular for molecular systems which cannot be treated quantum mechanically, and it opens perspectives for a variety of other systems involving complex molecules (e.g., O_2-H_2O, CH_4-H_2O, ...). Finally, the fact that the air humidity must be taken into account for accurate predictions of atmospheric spectra (and associated retrieval exercises) around 4 μm is demonstrated using measurements of transmissions from ground and of radiances from space.

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[1] J.-M. Hartmann, et al., *J. Chem. Phys.*, 148, 054304 (2018).

[2] Y. Baranov, et al., *Phil. Trans. R. Soc. A*, 370, 2691-709 (2012).

[3] H. Tran, et al., *Icarus*, 306, 116-21 (2018).

[4] J.-M. Hartmann, et al., *J. Geophys. Res. Atmos.*, 122, 2419-28 (2017).

[5] J.-M. Hartmann, et al., *J. Chem. Phys.*, 134, 184312 (2011).

VII-8. Near-Infrared Water Vapour Continuum Derived from Sun-Pointing FTS Measurements

J. Elsey,[a] K. P. Shine,[a] M. D. Coleman,[b] T. Gardiner [b]

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The water vapour continuum is the smoothly-varying wavelength-dependent absorption not attributable to local spectral lines of the water vapour molecule. This absorption is weak in comparison to line absorption; however in the near-infrared windows at 2.1 and 1.6 μm it is the largest gaseous contributor to atmospheric absorption and is important in radiative transfer applications both for energy budget and climate studies, and for remote sensing using these windows.

While it is currently parameterised in models (usually using the MT_CKD continuum), its strength and temperature dependence are not well constrained. Laboratory observations of the self-continuum near room temperature differ by a factor of around 100 in the centre of the 1.6 μm window and by a factor of 5 to 10 near the centre of the 2.1 μm window[1], with no agreement within the respective measurement uncertainties. These laboratory measurements are taken at or above room temperature; given the difficulty in extrapolating these measurements to lower temperature, the true continuum strength in the atmosphere is even more difficult to ascertain.

This work presents an analysis aiming to extract the continuum strength from atmospheric measurements made by the UK National Physical Laboratory, using an absolutely calibrated sun-pointing Fourier Transform Spectrometer; these measurements have recently been used to improve estimates of the near-IR extraterrestrial solar spectral irradiance[2]. Deriving the continuum is a more challenging task, due to the need to correct for aerosol scattering, time-varying water vapour amounts and measurement uncertainties. Despite these uncertainties, we find a continuum strength in these windows with central values larger than those predicted by MT_CKD. Advances that will be needed to better constrain the uncertainty in the near-infrared continuum in future atmospheric measurements will also be discussed.

---

[1] K. P. Shine, et al., *J. Molec. Spec.*, 327, 193-208 (2016).

[2] J. Elsey, M. D. Coleman, T. Gardiner, K. P. Shine, *Geophys. Res. Lett.*, 44, 10071-10080 (2017).

VII-9. Accurate Measurements of Weak Absorption Continua of H_2O, CO_2 and O_2 by Cavity-Enhanced Spectroscopic Techniques

D. Mondelain,[a] **A. Campargue**,[a] **R. Grilli**,[b] **S. Kassi**,[a] **L. Lechevallier**,[b]
L. Richard,[a] **D. Romanini**,[a] **S. Vasilchenko**,[a] **I. Ventrillard**[a]

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Since now few years we are involved in the determination of continua of atmospheric species (i.e., H_2O, CO_2 and O_2) in the infrared by cavity-enhanced spectroscopy techniques. Thanks to their sensitivity and base line stability these techniques, cavity ring down spectroscopy (CRDS) and optical feedback cavity-enhanced absorption spectroscopy (OF-CEAS), are perfectly adapted to measure weak absorptions slowly varying with frequency.

Using a variety of laser sources, the water vapor self-continuum cross-sections was accurately determined by CRDS and OF-CEAS in the transparency windows centered around 4.0, 2.1, 1.6 and 1.25 μm[1]. The corresponding cross-sections were derived either from the baseline variation of water vapor spectra recorded for a series of pressure values over a small spectral interval or from baseline monitoring at fixed laser frequency during pressure ramps. After subtraction of the local water monomer lines contribution, the measurements provide a unique set of cross-sections which has been used to adjust the last version (3.2) of the semi-empirical MT_CKD model (Mlawer-Tobin_Clough-Kneizys-Davies), widely incorporated in atmospheric radiative-transfer codes. Temperature dependence of the absorption continuum was also measured in the 23-50°C range for a few spectral points and compared to literature values.

Recently we have started to investigate the collision induced absorption (CIA) coefficients of the $a^1\Delta_g$–$X^3\Sigma_g^-$ band of oxygen near 1.27 μm. More precisely, the B_{O2-O2}, B_{O2-N2} and B_{O2-Air} coefficients have been determined with a reduced uncertainty from series of low density spectra (from 0.36 to 0.85 amagat) of pure oxygen and N_2+O_2 mixture with O_2 relative abundance of 20.95%. CIA is obtained from the difference between the absorbing samples spectra and argon spectra recorded for the same densities after removal of the local contribution of the absorption lines. The low densities at which the spectra are recorded are very useful to reliably remove this local contribution. The retrieved coefficients are compared to the CIA reported in Maté et al.[2] A good overall agreement is found but differences between 5 to 8% are observed for B_{O2-Air} below 7850 m^{-1}.

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[1] L. Lechevallier, et al., *Atmos. Meas. Tech.*, 11, 1-13 (2018).

[2] B. Maté et al., *J. Geophys. Res.*, 104, 30585-30590 (1999).

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HITRAN Anthem

As sang at Larry Rothman's retirement party in May 2017

(Music from "If You're Happy and You Know It")

It's the spectral database - It's called HITRAN
It is used from San Francisco to Milan
It is used in the US, and in Russia and in France

Everybody use HITRAN, HITRAN, HITRAN

If you want to find a leak in your gas pipe
Or you want to find a non-terrestrial life
Or check pollution at your plant, that is when you use HITRAN

Everybody use HITRAN, HITRAN, HITRAN

To detect an early cancer in the breath
Or to see if someone bakes the crystal meth
You should make a proper plan: How to use HITRAN, HITRAN

Everybody use HITRAN, HITRAN, HITRAN

What about that nasty ozone hole?
Is it shrinking over the North Pole?
You should check the database, against what you see from space

Everybody use HITRAN, HITRAN, HITRAN

Larry Rothman made it so much fun
When we use the spectra from HITRAN
It is such a useful tool, and we all say big THANK YOU

And we all say big THANK YOU, THANK YOU, THANK YOU

CONFERENCE PROGRAM
DAY 1, Wednesday 13 June

07:30 Registration and breakfast

08:30 WELCOME ... I. E. Gordon and L. S. Rothman

SESSION I: Databases and Tools

Chair: L. S. Rothman

08:50 **I-1.** Brief Report on the Status and Future Directions of the HITRAN Database ... I. E. Gordon

09:05 **I-2.** Considerations for Sharing and Preserving Research Software and Data ... D. Bouquin

09:35 **I-3.** PNNL Databases for Atmospheric Monitoring ... T. J. Johnson

10:15 *Coffee Break* ...

10:35 **I-4.** Spectroscopic Toolbox for HITRAN ... R. V. Kochanov

11:15 **I-5.** Evaluation of the Spectroscopic Parameters of Current Spectroscopic Databases, such as GEISA-2015 and HITRAN-2016, in the Frame of the New 2018 Release of GEISA ... R. Armante

11:30 **I-6.** MODTRAN6 Line-By-Line Algorithm ... A. Berk

11:45 **I-7.** Spectroscopic Databases for the VAMDC Portal: New Tools and Improvements ... C. Richard

12:00 ICAMDATA conference announcement ... N. Brickhouse

12:05 *Lunch Served* ...

SESSION II: Planetary-Relevant and High-Temperature Spectroscopy

Chair: J. Tennyson

13:30 *Brault Award Ceremony* ...

13:35 **II-1.** High Temperature Laboratory Measurements, Atmospheric Retrievals, and Future Plans for HITEMP ... R. J. Hargreaves

14:15 **II-2.** Frequency Comb Lasers in High-Temperature Spectroscopy: Spectral Database Development to Practical Field Measurements ... G. B. Rieker

14:55 **II-3.** Laboratory Spectroscopy for Exoplanets ... P. F. Bernath

15:10 **II-4.** Line Positions and Intensities for the ν_3 Band of 5 Isotopologues of Germane for Planetary Applications ... V. Boudon

15:25 **II-5.** Water Vapor: Line Intensity Study of ^{18}O Enriched Spectra Between 6450 and 8000 cm^{-1} and H_2O Line Shape Parameters Broadened by CO_2 ... L. Régalia

15:40 **II-6.** Line Positions and Intensities in the 7400–8600 cm^{-1} Region of the Ammonia Spectrum ... J. Vander Auwera

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

DAY 2, Thursday 14 June
SESSION III: Exoplanets and Stars

Chair: C. Sousa-Silva

08:45 **III-1.** Characterization of Exoplanet Atmospheres via Molecular and Atomic Spectroscopy ... A. Oklopčić

09:25 **III-2.** The Calculation of Atomic and Molecular Opacities for Astrophysical Applications ... R. Freedman

10:05 **III-3.** Planetary Spectrum Generator: An Accurate Online Radiative Transfer Suite for Atmospheres, Comets, Small Bodies and Exoplanets ... G. L. Villanueva

10:20 **III-4.** Fast Spectral Synthesis for a New Generation of Solar and Stellar Brightness Variability Models ... M. Cernetic

10:35 Twinkle mission in 5 minutes ... J. Tennyson

10:40 *Coffee Break* ...

SESSION IV: Theoretical Linelists for Exoplanets

Chair: M. Rotger

10:55 **IV-1.** The ExoMol Project: Progress and Perspectives ... J. Tennyson

11:15 **IV-2.** TheoReTs – *Ab Initio* Based Information System For Astrophysical Applications: Line Lists, Cross-Sections And Validation Versus Observed Spectra ... V. Tyuterev

11:35 **IV-3.** The Spectroscopy of C_3: New Challenges and New Physics ... D. W. Schwenke

11:55 **IV-4.** Molecular Simulations for the Spectroscopic Detection of Biosignature Gases and Other Volatiles ... C. Sousa-Silva

12:10 **IV-5.** Sub-percent accuracy for the intensities of top five HITRAN molecules ... O. L. Polyansky

12:25 *Lunch Served and Group Photo* ...

SESSION V: Spectroscopy of the Terrestrial Atmosphere

Chair: P. F. Bernath

13:30 *Benedict Award Ceremony* ....

13:35 **V-1.** Atmospheric Spectroscopy at the Smithsonian Astrophysical Observatory: From Mount Sinai to Geostationary Orbit and Beyond .... K. Chance

14:15 **V-2.** Spectroscopy for Remote Sensing of Tropospheric Composition: Perspectives from the Aura-TES and OCO-2 Teams .... V. H. Payne

14:55 **V-3.** Re-evaluating the Use of O_2 $a^1\Delta_g$ Band in Spaceborne Remote Sensing of Greenhouse Gases .... K. Sun

15:10 *Coffee Break* ....

15:30 **V-4.** Satellite Remote Sensing of the Atmosphere: Past (MIPAS) and Future (FORUM) Challenges .... B. M. Dinelli

16:10 **V-5.** Spectroscopy Issues for the Atmospheric Chemistry Experiment .... C. D. Boone

16:25 **V-6.** CO_2 Spectroscopy and Forward Modelling Accuracy in the Thermal Band: An Assessment Study with IASI Spectral Observations . G. Masiello

16:40 **V-7.** Evaluating Different HITRAN Databases Using AIRS and CrIS .... S. DeSouza-Machado

16:55 **V-8.** Low-Temperature, High-Precision Measurements of the O_2 A-Band .... E. M. Adkins

17:10 **V-9.** Multispectrum Analysis of the Oxygen A-Band .... B. J. Drouin

18:30 *Conference Banquet* ....

DAY 3, Friday 15 June
SESSION VI: Laboratory Measurements

Chair: M. A. H. Smith

08:45 **VI-1.** Recent Progress in the Infrared Spectroscopy of Ozone .... A. Barbe

09:25 **VI-2.** New Spectroscopic Data for Tropomi/S5P in the 2.3 μm region for CH_4 and H_2O and a New UV Database for Ozone .... M. Birk

10:05 **VI-3.** New absolute and relative line intensities of ozone fundamentals - a step towards the end of the ozone UV/MIR dilemma .... G. Wagner

10:20 **VI-4.** Measurements of Ozone Line Intensities at 5 and 10 μmD. Jacquemart

10:35 *Coffee Break* ....

10:55 **VI-5.** Comb-Assisted CRDS of Water Vapor: From Extensive Spectral Coverage to Doppler-Free Saturation Dips .... A. Campargue

11:10 **VI-6.** Investigation of the ν_8 and ν_{21} Bands of Propane at 11.5 and 10.9 μm: Evidence of Large Amplitude Tunnelling Effects .... A. Perrin

11:25 **VI-7.** Quantitative Infrared Spectroscopy of Halogenated Species for Atmospheric Remote Sensing .... J. J. Harrison

11:40 **VI-8.** Precise Line Positions from Laser-Locked Cavity Ring-Down Spectroscopy .... S.-M. Hu

11:55 **VI-9.** Molecular Line Intensities of Carbon Dioxide in the 1.6 μm Region Determined by Cavity Ringdown Spectroscopy .... Z. D. Reed

12:10 **VI-10.** Towards a Coherent Spectral Line Parameter Set for the Complete $2\nu_3$-Band of $^{14}N_2{}^{16}O$ Using High Resolution FTIR-Spectroscopy . V. Ebert

12:25 *Lunch Served* ....

SESSION VII: Lineshapes and Continua

Chair: J. T. Hodges

13:30 **VII-1.** Line-Shape Problems in Modelling Laboratory and Atmospheric Spectra and Predictions of High-Order Line-Shape Parameters using Molecular Dynamics Simulations .... H. Tran

14:10 **VII-2.** First Comprehensive Dataset of Beyond-Voigt Line-Shape Parameters from *Ab Initio* Quantum Scattering Calculations for the HITRAN Database .... P. Wcisło

14:25 **VII-3.** Temperature Dependence of Half-Widths and Line Shifts for Molecular Transitions in The Microwave and Infrared Regions .... R. R. Gamache

14:40 **VII-4.** Line Shape Parameters for the 1←0 Bands of CO Isotopologues .... M. A. H. Smith

14:55 *Coffee Break* ....

15:15 **VII-5.** Recent Enhancements to the MT_CKD Continuum: Part I .... E. J. Mlawer

15:30 **VII-6.** Recent Enhancements to the MT_CKD Continuum: Part II .... M. J. Alvarado

15:45 **VII-7.** Influence of Humidity on Absorption by N_2 and CO_2 Near 4 μm: Calculations, Comparisons with Measurements and Atmospheric Consequences .... J.-M. Hartmann

16:00 **VII-8.** Near-Infrared Water Vapour Continuum Derived from Sun-Pointing FTS Measurements .... K. P. Shine

16:15 **VII-9.** Accurate Measurements of Weak Absorption Continua of H_2O, CO_2 and O_2 by Cavity-Enhanced Spectroscopic Techniques .... D. Mondelain

16:30 *Close* ....