



HITRAN spectroscopy evaluation using solar occultation FTIR spectra



Geoffrey C. Toon^{a,*}, Jean-Francois Blavier^a, Keeyoon Sung^a,
Laurence S. Rothman^b, Iouli E. Gordon^b

^a Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States

^b Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, United States

ARTICLE INFO

Article history:

Received 22 April 2016

Received in revised form

22 May 2016

Accepted 22 May 2016

Available online 11 June 2016

Keywords:

Spectroscopy

Infrared

Atmosphere

Remote Sensing

HITRAN

ABSTRACT

High resolution FTIR solar occultation spectra, acquired by the JPL MkIV Fourier transform spectrometer from balloon, covering $650\text{--}5650\text{ cm}^{-1}$ at 0.01 cm^{-1} resolution, are systematically analyzed using the last four versions of the HITRAN linelist (2000, 2004, 2008, 2012). The rms spectral fitting residuals are used to assess the quality and adequacy of the linelists as a function of wavenumber and altitude. Although there have been substantial overall improvements with each successive version of HITRAN, there are nevertheless a few spectral regions where the latest HITRAN version (2012) has regressed, or produces residuals that far exceed the noise level. A few of these instances are investigated further and their causes identified. We emphasize that fitting atmospheric spectra, in addition to laboratory spectra, should be part of the quality assurance for any new linelist before public release.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

The HITRAN linelist [19] is without doubt the most widely used spectroscopic database and underpins most atmospheric remote-sensing experiments. As our understanding of the terrestrial atmosphere improves, the accuracy required of new measurements becomes more stringent. Hence the requirements on the accuracy and completeness of the spectroscopy become inexorably more challenging.

It is usually impossible to fit high-resolution Infra-Red solar spectra (high SNR) down to their noise level, at least below 25 km tangent altitude. Residuals are typically dominated by systematic errors arising from defects in the assumed atmospheric temperature (T), pressure (P), and volume mixing ratio (vmr) profiles, the observation geometry (pointing), the instrumental response (e.g., instrument line

shape, zero-level-offsets, channel fringes, phase errors, aliasing, ghosts), and spectroscopic inadequacies. For spectra measured with a well-calibrated instrument under well-known atmospheric conditions, the first three types of systematic errors can usually be minimized, revealing the underlying spectroscopic problems.

In the past we successfully used the Total Carbon Column Observing Network (TCCON) Fourier Transform Spectrometer (FTS) in Park Falls, WI for validating spectroscopic parameters of molecular oxygen in different spectral windows [5,6]. In the first paper not only the parameters of strong magnetic dipole lines in the $1.27\text{ }\mu\text{m}$ band were validated but the electric quadrupole lines were identified for the first time in this band. Previously they were thought to be orders of magnitude weaker. Similar evaluations were done in limited spectral regions of water, methane and carbon dioxide prior to the release of the HITRAN 2012 database.

In this paper, we document the quality of fits to atmospheric spectra collected by the JPL MkIV interferometer and

* Corresponding author.

E-mail address: Geoffrey.C.Toon@jpl.nasa.gov (G.C. Toon).

fitted using the JPL Gas Fitting software (GFIT), to provide a benchmark for assessment of future linelists (e.g., HITRAN 2016) and to highlight gases and spectral regions where further spectroscopic work would be beneficial.

2. MkIV instrument

The MkIV FTS is a double-passed FTIR spectrometer designed and built at JPL in 1984 for atmospheric observations [21]. It covers the entire $650\text{--}5650\text{ cm}^{-1}$ region simultaneously with two detectors: a HgCdTe photoconductor covering $650\text{--}1800\text{ cm}^{-1}$ and an InSb photodiode covering $1800\text{--}5650\text{ cm}^{-1}$. The MkIV instrument has flown 24 balloon flights since 1989. It has flown on over 40 flights of the NASA DC-8 aircraft as part of various campaigns during 1987–1992 studying high-latitude ozone loss. It has also made over 1100 days of ground-based observations since 1985 (covering three full solar cycles) from a dozen different sites, from Antarctica to the Arctic, from sea-level to 3.8 km altitude.

3. Balloon spectra

A solar occultation of balloon spectra measured by the JPL MkIV FTS over Alaska in May 1997 was used for this work. This particular balloon flight was chosen because it was part of the Photochemistry of Ozone Loss in the Arctic Region In Summer (POLARIS) campaign [10], which aimed to study the summertime ozone depletion from NO_x chemistry. In addition to balloon flights, the NASA ER-2 aircraft made dozens of flights over Alaska. There were also frequent ground-based remote-sensing observations (e.g. [22]). Thus the atmosphere over Alaska was exceptionally well characterized during this period. For example, the MkIV balloon profiles of various atmospheric gases were compared with coincident in situ measurements by instruments on board the NASA ER-2 aircraft [23].

The MkIV balloon spectra cover the $650\text{--}5650\text{ cm}^{-1}$ region at 0.01 cm^{-1} resolution and tangent altitudes from 10 to 38 km. The sunrise spectra used in this study were ratioed by a MkIV high-sun (35° solar zenith angle) spectrum measured around solar noon from 39 km altitude during a Sep 1996 balloon flight. Since the MkIV instrument was unchanged between these two flights, and the Mid Infra-Red (MIR) solar spectrum changes little over 8 months, the ratioing removes spectral features arising from the sun or the instrument.

4. Spectral fitting methodology

The balloon spectra were fitted using the four latest versions of the HITRAN linelist: HITRAN 2000 [17], HITRAN 2004 [16], HITRAN 2008 [18], and HITRAN 2012 [19]. For gases not present in the main HITRAN linelist, but for which measured absorptions coefficients are provided on the HITRAN website (e.g., CFC-11, CFC-12, HCFC-22, etc.), pseudo-line-lists derived from those absorption spectra were used [<http://mark4sun.jpl.nasa.gov/pseudo.html>]. These derived pseudo-line-lists were unchanged between

the four HITRAN versions, as was everything else (spectra, software, atmospheric models, etc.). So the differences in the spectral fits result solely from changes to the line-by-line portion of HITRAN.

The spectral fitting was performed with the GFIT code, a non-linear least-squares algorithm developed at JPL that scales the atmospheric gas volume mixing ratios (vmrs) to fit calculated spectra to those measured. For balloon observations, the atmosphere was discretized into 100 layers of 1 km thickness. Absorption coefficients were computed line-by-line assuming a Voigt lineshape. The line mixing option was not used in this work.

Sen et al. [20] provide a more detailed description of the use of the GFIT code for retrieval of vmr profiles from MkIV balloon spectra. GFIT was previously used for the Version 3 analysis [7] of spectra measured by the Atmospheric Trace Molecule Occultation Spectrometer (ATMOS), and is currently used for analysis of TCCON spectra [26].

Fig. 1 lists the 112 fitted windows, and the adjusted gases in each. Gases not listed (e.g. O_2) are still included in the calculation, but their vmr profile is not adjusted. Isotopologues are given different a priori vmr profiles to account for any atmospheric fractionation. A frequency shift was also fitted for each window, which means that line position errors affecting an entire window will not impact the Root Mean Squared (rms) fitting residuals. However, line position errors specific to particular transitions, or which differ between overlapping bands of different gases, will increase the rms residual. We note that these windows are broader than those currently adopted by the Network for Detection of Atmospheric Change Infra-Red Working Group (NDACC IRWG) in the MIR, but similar to those used by TCCON in the Near Infra-Red (NIR). The MIR windows are generally narrow to avoid troublesome interfering features, but we expect them to be widened in the future as the spectroscopy improves.

5. Results

Fig. 1 shows the rms spectral residuals (observed - calculated) achieved for each window, plotted versus the central wavenumber of that window. Three sample tangent altitudes are illustrated: 10, 20 and 31 km. The size of the horizontal-bars represents the width of the fitted window. In total, 112 windows were fitted across the $670\text{--}5600\text{ cm}^{-1}$ region, with widths ranging from 4 to 114 cm^{-1} , the broader windows being necessary to bridge across regions, such as the ν_3 band of CO_2 which is completely saturated at lower altitudes. The different colors represent the four different linelists. In windows where there was no change in the rms, intermediate colors are seen (e.g., orange+green=brown). The top panel shows results from 31 km tangent altitude. Here the lowest rms values represent the measurement noise and are found in "window" regions where absorption is very weak e.g., $800\text{--}950$, $1150\text{--}1250$, and $2400\text{--}2700\text{ cm}^{-1}$. The bottom panel represents 10 km altitude. Here the smallest rms residuals are found in a few saturated regions (i.e., no photon flux), e.g. $660\text{--}740$, $1500\text{--}1600$, $2200\text{--}2400$, and $3700\text{--}3900\text{ cm}^{-1}$. The largest residuals occur at altitudes

Download English Version:

<https://daneshyari.com/en/article/5427562>

Download Persian Version:

<https://daneshyari.com/article/5427562>

[Daneshyari.com](https://daneshyari.com)