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Measured and simulated absorption of CO_2 at high pressure and temperature: a new tool for remote sensing instruments

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Abstract

Here we present a comparison between measured and calculated absorption of CO_2 gas at extreme conditions as found in the deep Venusian atmosphere. In addition, we describe a new tool to reproduce the absorption of CO_2 with state of the art theory, in order to support remote sensing studies by instrumentation on orbiting spacecraft. Gas transmittance spectra have been recorded by a Fourier Transform InfraRed (FT-IR) spectrometer covering a wide spectral range, from 350 to 25000 cm^{-1} (0.4 to 29 μm) with a spectral resolution from 10 to 0.07 cm^{-1}. A special customized gas cell, certified to support pressures up to 350 bar and temperatures up to 300° C, has been integrated inside a compartment of the interferometer. A large number of spectra has been recorded on a pressure-temperature grid from 1 to 30 bar and 298 to 600 K. Our experimental spectra have been compared with synthetic spectra obtained by a software that takes into account line-mixing due to inter-molecular collisions. Inclusion of the line mixing, which is depending on the molecular density, produces spectra which differ substantially from those produced by simpler models, (such as ARS [3]) using a Voigt profile and neglecting line mixing, in particular for the high pressure and temperature conditions present in the Venus' atmosphere.

1. Introduction

The widely used spectroscopic databases, like HITRAN, HITEMP, CDSD, contain a wealth of spectroscopic data, including absorption coefficients of most isotopic species of carbon dioxide, as well as line broadening parameters for a limited number of bands. While these data allow for a satisfactory simulation of the Earth atmosphere, the particular conditions of high pressure and temperature of the Venus' atmosphere require a more sophisticated theoretical model and in some cases molecular parameters. While extensive data sets exist for radiative transfer calculations concerning the Earth's atmosphere, important information and a thorough understanding of the behaviour of dense planetary atmospheres is still missing. Presently the availability of extended datasets produced by remote sensing instruments, in particular by the Visible and InfraRed Thermal Imaging Spectrometer (VIRTIS) instrument on board Venus Express, requires an additional effort to better reproduce the radiance coming from the deep atmosphere of Venus. This effort translates in a better accuracy of the retrieved abundance of minor species or the capability to retrieve the physical conditions at a lower altitude, as close as possible to the surface. In order to test the ability of sophisticated models in reproducing transmission spectra in Venus' conditions, we've assembled an experimental setup to produce spectra which allow us to characterize and model the optical properties of CO_2.

2. Results

We reproduced in our cell the real Venusian physical conditions for CO_2 in a grid from the VIRA profile [1], varying the CO_2 pressure from 1 to 30 bar and temperature from 298 to 600K. For each point of the grid we measured the absorbance of the gas (see figure 1). The grid represents the same conditions found in the deep atmosphere of Venus from an altitude of 50 Km down to 15 km. The measurements have been compared with synthetic spectra produced according to the method described in [2], which takes into account line-mixing effects for all bands present in the spectral region considered (from 800 to 10000 cm^{-1}). In figure 2 an example of the comparison is shown. In spectral regions with very strong absorption also the far wings have been taken into account, by using an empirical model using χ correction factors .

3.Figures

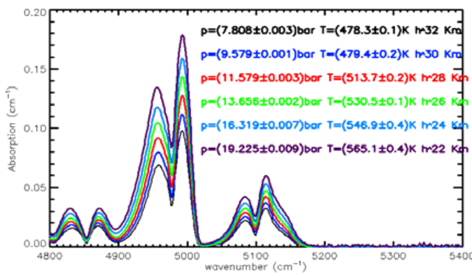

Figure1: CO_2 absorption coefficients measured at different pressure and temperature.

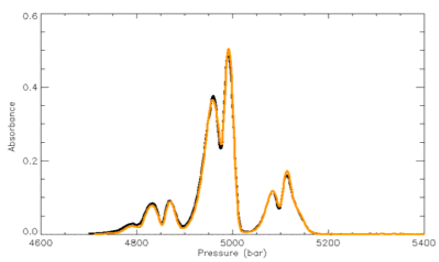

Figure 2: Comparison between Measured (black curve) and simulated (orange curve) at p = 40bar and T= 373K

4 . Conclusions

The CO_2 spectra have been measured for a wide range of temperatures and pressures for a large spectral range. A theoretical model including line mixing effects as well as far wings corrections for the strongest absorption bands reproduces the laboratory spectra excellently, for all pressures and temperatures. Simpler models, such as ARS [3], neglecting line mixing and far wings, and using Lorentz or Voigt line shapes have shown to be inadequate to reproduce carbon dioxide absorption in the Venusian atmosphere. For the far wings region, sets of temperature dependent χ factors have been constructed for the ν2, ν3 and ν1+ν3 bands wing regions ([2]).

In our approach the collision induced absorption (CIA) has been neglected. Further work is going on in order to include the CIA, by using a semi-empirical model, based on laboratory spectra of collision induced absorption bands.

References

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