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Measurements of CO₂ line parameters in the 9250–9500 cm⁻¹ and 10,700–10,860 cm⁻¹ regions



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ABSTRACT

The absorption spectra of carbon dioxide have been recorded in two wavenumber ranges 9250–9500 cm⁻¹ and 10,700–10,860 cm⁻¹ of the near infrared region using a Bruker IFS 125 HR Fourier transform spectrometer and a 30 m multipass cell with the White type optical system. The spectra were recorded at spectral resolution of 0.03 cm⁻¹, room temperature, path length of 726.7 m and at four pressures ranging from 187 to 674 mbar. The achieved sensitivity (noise equivalent absorption) at the level of $k_{\nu} = 7.2 \times 10^{-10}$ cm⁻¹ allowed detection of numerous new transitions with intensity values down to 5×10^{-29} cm/molecule. The respective measurement time is about 20 h. The multi-spectrum fittings with the Voigt profile were performed to retrieve the line positions and intensities of 12 observed bands. Three hot bands of ¹²C¹⁶O₂ in the 9250–9500 cm⁻¹ region were detected for the first time. The line intensities of 30032–00001 and 30033–00001 bands of ¹²C¹⁶O₂ and of 20032–00001 band of ¹⁶O¹²C¹⁸O were measured for the first time.

The uncertainty of the line position determination is estimated to be about 0.001 cm⁻¹ for the unblended lines with high value of signal-to-noise ratio. The uncertainty of the line intensity determination varies from 5% to 40% depending on the line strength and on extent of line overlapping. The measured line intensities of 30032–00001 and 30033–00001 bands together with those published for the 00051–00001 band were used to fit the effective dipole moment parameters of ¹²C¹⁶O₂ for the $\Delta P = 15$ series of transitions, where $P = 2V_1 + V_2 + 3V_3$ is a polyad number (V_i ($i = 1, 2, 3$) are vibrational quantum numbers). The fitted parameters reproduce the measured line intensities within experimental uncertainties. Comparison of the measured line positions and intensities to those contained in HITRAN, GEISA, CDSD and AMES line lists is given.

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1. Introduction

In this paper we have revisited the 9250–9500 cm^{-1} (1.05–1.08 μm) and 10,700–10,860 cm^{-1} (0.92–0.93 μm) regions of the CO_2 spectrum using a Bruker IFS 125 HR Fourier transform spectrometer (FTS) and a 30 m multipass cell with the White type optical system at the V.E. Zuev Institute of Atmospheric Optics [1]. These regions could be used for the investigation of the chemical and isotopic compositions of Venus and Mars atmospheres [2,3].

The 9250–9500 cm^{-1} spectral region was previously studied in the Refs. [4–11]. Absorption in this region is dominated by the 20032–00001, 20033–00001, 21132–01101, 21133–01101 bands of $^{12}\text{C}^{16}\text{O}_2$ and the 20032–00001, 20033–00001 bands of $^{13}\text{C}^{16}\text{O}_2$, as it is shown in Fig. 1, where data from the CDSD-296 databank [12] are used. In our recent paper [11] spectra in this region were recorded using the 30 m base length multipass cell, which provided a 612.26 m path length. The line positions and intensities of the 20032–00001, 20033–00001 and 21132–01101 bands of $^{12}\text{C}^{16}\text{O}_2$ were reported. Nowadays our setup allows using longer path lengths, and therefore higher sensitivity could be reached. Because of that we decided to repeat the spectra recording in this spectral region trying to detect new hot bands and bands of less abundant carbon dioxide isotopologues.

Two bands 30032–00001 and 30033–00001 of Fermi tetrad 3003*i*–00001 (*i*=1,2,3,4) of $^{12}\text{C}^{16}\text{O}_2$ dominate in the 10,700–10,860 cm^{-1} region. The Fermi tetrads of $^{12}\text{C}^{16}\text{O}_2$ and $^{13}\text{C}^{16}\text{O}_2$ have been studied with ICLAS technique [13]. Line positions were measured with estimated uncertainty 0.005 cm^{-1} . The estimates of the integrated band intensities of these bands were also done in the cited paper. But to our knowledge no any line intensity measurements have been performed for these bands.

2. Experimental details

The absorption spectra of carbon dioxide with natural isotopic abundance have been recorded using the Bruker IFS 125 HR FTS and the 30 m base length multipass cell at the V.E. Zuev Institute of Atmospheric Optics (Tomsk). The cell is equipped with the White type three mirrors optical system. In comparison to our previous measurements [11] in this study we used mirrors covered with silver which have the reflectance coefficient of about 98% in visible and near IR regions. The FTS and the cell alignment allowed us to effectuate 26 passes of a ray inside the cell, which gives the path length of 726.7 m at a basic distance between mirrors of 27.95 m. This path length was gained with utilization of a halogen lamp of 50 W as a light source and a diaphragm of 1.3 mm. More detailed description of this setup is given in Ref. [1].

Before the measurements the cell was pumped out to a pressure of 80 mbar using a rotary water ring pump, and then with three vacuum pumps it was pumped out to a pressure of 5×10^{-3} mbar. To avoid any pressure and temperature instability inside large volume of the cell we filled it with CO_2 slowly during 2 h and the experiments were conducted 3 h after the filling. The spectra were recorded in two spectral

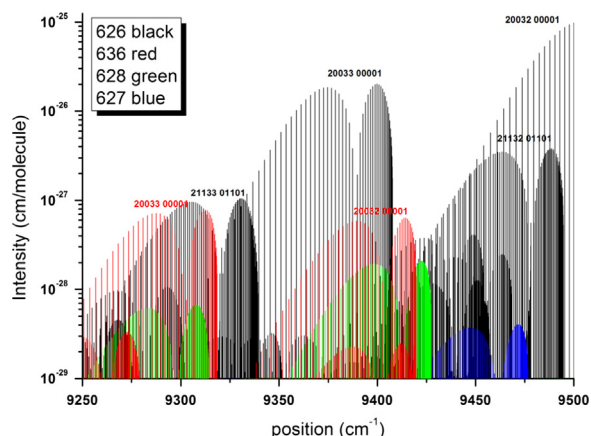


Fig. 1. Stick spectrum of natural carbon dioxide in the 9250–9500 cm^{-1} spectral region according to the CDSD database [12]. (For interpretation of an isotopologue to color in this figure legend, the reader is referred to the web version of this article.)

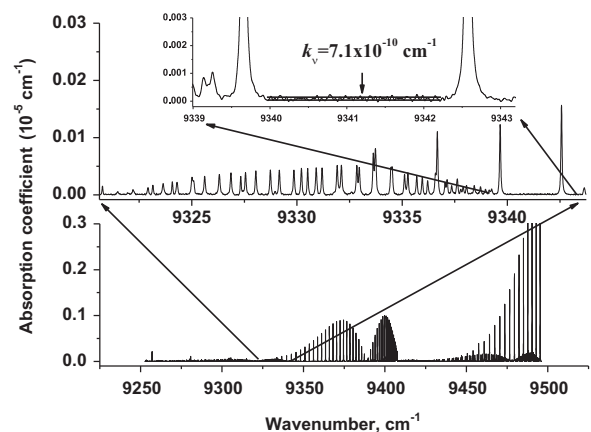


Fig. 2. Fourier transform spectrum of carbon dioxide in the 9250–9500 cm^{-1} region ($P=297$ mbar, $L=726.7$ m, $T=2.89$ K). The insets displayed on the upper panels illustrate the high sensitivity of the recordings (noise equivalent absorption is an order of 7.2×10^{-10} cm^{-1}).

regions 9340–9650 and 10,700–10,860 cm^{-1} with unapodized resolution 0.03 cm^{-1} at temperature 289 K using CO_2 sample of 99.9% purity with natural isotopic abundance. Si detector was used to record absorption spectra in both spectral regions. The pressure of CO_2 varying from 187 mbar to 674 mbar was measured with a DVR-5 capacitance manometer (1100 mbar full scale) with a stated uncertainty of ± 1 mbar according to manufacturer. Four absorption spectra of CO_2 have been recorded in this pressure range at 187, 297, 469 and 674 mbar. The temperature was measured by three thermocouples installed on the body of the cell. The minimal detectable absorption coefficient k_v was 7.2×10^{-10} cm^{-1} in the 9250–9500 cm^{-1} region (as it is illustrated in Fig. 2) and 5×10^{-9} cm^{-1} in the 10,700–10,860 cm^{-1} region. This was achieved by coaddition of 2000 interferograms and utilization of the filters during the measurements. The experimental conditions are summarized in Table 1.

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