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High sensitivity *CW*-Cavity Ring Down Spectroscopy of five $^{13}CO_2$ isotopologues of carbon dioxide in the 1.26–1.44 μm region (I): Line positions

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ABSTRACT

The absorption spectrum of highly enriched ^{13}C carbon dioxide has been investigated by CW-Cavity Ring Down Spectroscopy with a setup based on fibered distributed feedback (DFB) laser diodes. By using a series of 30 DFB lasers, the CO_2 spectrum was recorded in the 7029–7917 cm^{-1} region with a typical sensitivity of 3×10^{-10} cm^{-1}. The uncertainty on the determined line positions is on the order of 8×10^{-4} cm^{-1}. More than 3800 transitions with intensities as low as 1×10^{-29} cm/molecule were detected and assigned to the $^{13}C^{16}O_2$, $^{16}O^{13}C^{17}O$, $^{16}O^{13}C^{18}O$, $^{17}O^{13}C^{18}O$ and $^{13}C^{18}O_2$ isotopologues. For comparison, only 104 line positions of $^{13}C^{16}O_2$ were previously reported in the literature in the considered region. The band-by-band analysis has led to the determination of the rovibrational parameters of a total of 83 bands including 56 bands of the $^{13}C^{16}O_2$ species. The measured line positions of $^{13}C^{16}O_2$ and $^{16}O^{13}C^{18}O$ were found in good agreement with the predictions of the respective effective Hamiltonian (EH) models but the agreement degrades for the minor isotopologues. Several cases of resonance interactions were found and discussed. In the 20033-10002 band of $^{13}C^{16}O_2$, an anharmonic resonance interaction leads to deviations on the order of 0.05 cm^{-1} compared to the EH predictions. The existence of interpolyad interactions affecting the non-symmetric isotopologues of carbon dioxide is confirmed by the observation of two occurrences in $^{16}O^{13}C^{17}O$ and $^{16}O^{13}C^{18}O$. The obtained results improve significantly the knowledge of the spectroscopy of the ^{13}C isotopologues of carbon dioxide. They will be valuable to refine the sets of effective Hamiltonian parameters used to generate the CDSD database.

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1. Introduction

The present work is devoted to the highly sensitive absorption spectroscopy of ^{13}C isotopologues of carbon dioxide. The high resolution spectra of such minor isotopologues are important in the studies of Venus and Mars atmospheres for which this gas is a principal constituent. The ground and satellite based infrared sensors used for these purposes work in the transparency windows of these atmospheres. Due to isotopic shifts and the change of the symmetry under isotopic substitution, the contribution of the minor isotopologues to the absorption in the transparency windows may largely exceed that of the principal isotopologue. Considering the large optical thicknesses the absorption of the minor isotopologues must then be accurately characterized. In addition, the knowledge of the corresponding concentrations is also important to understand the atmospheric physics of these planets [1–4].

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This contribution is part of the series of our publications devoted to the investigations of the absorption spectrum of carbon dioxide by high sensitivity CW-Cavity Ring Down Spectroscopy (CW-CRDS) in the spectral region accessible with distributed feedback (DFB) laser diodes. A first series of reports were devoted to natural carbon dioxide and ^{13}C enriched isotopologues in the 5851–7045 cm^{-1} region (1.71–1.42 μm) [5–12]. The achieved sensitivity allows detecting numerous new transitions with intensity down to 10^{-29} cm/molecule. In this 5851–7045 cm^{-1} region, the recent HITRAN2008 database [13] has adopted the CRDS line positions for the transitions below the detection limit (about 10^{-26} cm/molecule) of the measurements performed at Jet Propulsion Laboratory (JPL) by Fourier Transform Spectroscopy (FTS) [14–21]. Together with all the measurements available in the literature, these FTS and CRDS experimental values were used as input data in order to refine the parameters of the global effective Hamiltonian (EH) model and improve the theoretical Carbon Dioxide Spectroscopic Databank (CDSD) [22]. For the weak lines not present in the CRDS and JPL datasets and blended lines unobserved by CRDS due to overlapping with stronger lines, the HITRAN2008 line list [13] was completed with the CDSD line parameters down to an intensity cut off of 4×10^{-30} cm/molecule.

We have developed a second DFB laser CW-CRDS spectrometer dedicated to the 7000–7920 cm^{-1} range. It was applied for the first time to carbon dioxide in natural abundance [23,24]. A global list of 2881 lines was constructed for the four isotopologues contributing to the CRDS spectrum in the 7123–7917 cm^{-1} region. These CW-CRDS observations represented a significant improvement in terms of accuracy and sensitivity compared to Venus spectra (about 470 lines) [25] which were the main experimental source for line positions in the region. Some deviations between the observations and the CDSD calculations (used for HITRAN2008) were evidenced both for the line positions and line intensities. The measured line intensities allowed determining the ΔP=10 set of effective dipole moment parameters of $^{16}O^{12}C^{18}O$ and refining that of the ΔP=11 series of the principal isotopologue [24,26].

The present work is a very similar investigation devoted to the CW-CRDS spectrum of highly enriched ^{13}C carbon dioxide. The investigated spectral interval corresponds to a weak absorption region between the strong $3\nu_3$ band centered at 6780 cm^{-1} and the $\nu_1+3\nu_3$ dyad bands around 8000 cm^{-1}. Because the transitions are all weaker than 5×10^{-25} cm/molecule, in its 2004 version, the HITRAN database did not provide any $^{13}C^{16}O_2$ transition in our range. In its 2008 version, the HITRAN line list provided 1032 transitions which were all transferred from the theoretical Carbon Dioxide Spectroscopic Databank (CDSD). Previous observations relative to the ^{13}C isotopologues of carbon dioxide are very scarce: only 64 lines belonging to the 40012-00001 and 40013-00001 bands were identified in Venus spectra in the considered region [25]. This dataset was extended to 114 lines (belonging to the 40013-00001, 40012-00001, 11132-01101 bands) from FTS spectra recorded at USTC (Hefei) using a CO_2 sample with 99% enrichment in ^{13}C and a 105 m absorption path length [27]. The detection of 403 $^{13}CO_2$ lines in our CW-CRDS spectrum of carbon dioxide in natural isotopic abundance illustrates the higher sensitivity allowed by this technique. The line list provided as Supplementary Material attached to Ref. [23] includes these 403 transitions but the detailed analysis of the $^{13}CO_2$ bands was not reported as the present investigation performed with ^{13}C enriched sample provides a much more complete dataset. For instance, 2382 transitions of $^{13}C^{16}O_2$ and 1044 those of $^{16}O^{13}C^{18}O$ were identified in the present study.

After description of the experimental details (Section 2), the rovibrational assignment and the comparison with the EH predictions will be presented in Section 3. Section 4 will be devoted to the band by band fit and to the analysis of a number of *intra-* and *inter-* polyad interactions which were identified.

2. Experiment

The fibered DFB laser CW-CRDS spectrometer developed for the 7000–7900 cm^{-1} region is essentially identical to the one used in our previous studies [5–12] dedicated to the 5900–7000 cm^{-1} range. The reader is referred to Refs. [7,24,28,29] for the description of the experimental apparatus. The data acquisition has been updated compared to the first set up, leading to slightly better performances for both the sensitivity and wavenumber accuracy. The 7029–7917 cm^{-1} region was covered with the help of 30 fibered DFB lasers. The DFB typical tuning range is about 40 cm^{-1} by temperature tuning from −5 to 60 °C. The spectral coverage is complete except for a 3.5 cm^{-1} gap between 7897.2 and 7900.7 cm^{-1}. The stainless steel ringdown cell (l=2 m, Φ=10 mm) is fitted by a pair of super mirrors. Two sets of supermirrors were used. The first set used below 6610 cm^{-1}, leads to ringdown time varying smoothly from 50 to 70 μs according to the laser wavelength. The supermirrors used above 6610 cm^{-1} have a higher reflectivity ($\tau\sim150$ μs) allowing for an increased sensitivity. About one hundred ringdown events were averaged for each spectral data point, and about 6 min were needed in order to complete a temperature scan of one DFB laser. The corresponding noise level on the spectrum baseline varied from 5×10^{-10} to 1×10^{-10} cm^{-1}, depending on the ringdown time. Fig. 1 illustrates the achieved sensitivity and dynamic range on the intensity scale in the region of the 40012-00001 band: absorption coefficients ranging from $\alpha\sim4\times10^{-6}$ cm^{-1} down to the noise level at 3×10^{-10} cm^{-1} can be measured from the displayed spectrum.

The pressure (measured by a capacitance gauge) and the ringdown cell temperature were monitored during the spectrum recording. The pressure value was fixed to 13.3 hPa (10.0 Torr). The DFB linewidth is about one thousandth of the Doppler broadening leading to a mostly Gaussian line profile. The line centers were determined by using an interactive least squares multi-line fitting program assuming a line profile of Voigt-type. The fitting

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