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Infrared spectroscopy of ^{17}O- and ^{18}O-enriched carbon dioxide: Line positions and intensities in the 3200–4700 cm^{-1} region. Global modeling of the line positions of $^{16}O^{12}C^{17}O$ and $^{17}O^{12}C^{17}O$

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ABSTRACT

The line positions and intensities of carbon dioxide isotopologues have been retrieved in 3200–4700 cm^{-1} region from Fourier transform spectra of carbon dioxide recorded in LADIR (Paris, France) with the Bruker IFS 125-HR [Jacquemart D et al. J Quant Spectrosc Radiat Trans 2012;113:961–75]. In total 11318 line positions and intensities of 151 bands of 12 isotopologues $^{16}O^{12}C^{16}O$, $^{16}O^{13}C^{16}O$, $^{16}O^{12}C^{18}O$, $^{16}O^{12}C^{17}O$, $^{16}O^{13}C^{18}O$, $^{16}O^{13}C^{17}O$, $^{18}O^{12}C^{18}O$, $^{17}O^{12}C^{18}O$, $^{18}O^{13}C^{18}O$, $^{17}O^{12}C^{17}O$, $^{17}O^{13}C^{18}O$, and $^{17}O^{13}C^{17}O$ have been retrieved. 53 bands were newly assigned. All studied bands belong to the $\Delta P=5$ and $\Delta P=6$ series of transitions, where $P=2V_1+V_2+3V_3$ is the polyad number (V_i are the vibrational quantum numbers). The accuracy of the line position measurement is about 0.3×10^{-3} cm^{-1} for the unblended and not very weak lines. The accuracy of the line intensities varies from 4% to 15% depending on the isotopologue, on the intensity of the line and on the extent of the line overlapping. The spectroscopic constants for the majority of the observed bands have been derived. The observed line positions together with those collected from the literature were used to fit the effective Hamiltonian parameters for the $^{16}O^{12}C^{17}O$ and $^{17}O^{12}C^{17}O$ isotopologues. In both cases the fitted models were capable of reproducing the measured line positions with accuracy compatible with the measurement uncertainties (rms are 0.0011 cm^{-1} and 0.0009 cm^{-1} for $^{16}O^{12}C^{17}O$ and $^{17}O^{12}C^{17}O$, respectively). The observed intensities were used to fit the effective dipole moment parameters for the $\Delta P=5$ and $\Delta P=6$ series of transitions of $^{16}O^{12}C^{17}O$, $^{17}O^{12}C^{17}O$ and $^{16}O^{12}C^{18}O$ isotopologues of carbon dioxide.

1. Introduction

This paper continues the series of our publications devoted to the analysis of the spectra of carbon dioxide enriched with the 17 and 18 oxygen which were recorded in LADIR (Paris, France) and in USTC (Hefei, China) in the 1700–9000 cm^{-1} wavenumber region [1,2]. The aim of this research is to provide spectroscopic reference standards for the remote sensing of the planetary atmospheres of Mars, Venus and the Earth. The information about spectral line parameters of ^{17}OCO isotopologues contained in the existing databases HITRAN2008 [3], CDSD [4–6] and OCO [7] is not complete and needs to be validated because

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the majority of the parameters came from the calculations. The first paper of this series [1] is devoted to the establishing of the isotopic composition of the sample used in LADIR. In addition the line intensities of several bands of different isotopologues were measured for the first time. The second paper of the series [2] is mostly devoted to the assignment of the spectra recorded in LADIR and in USTC. The line positions were also determined in that paper with the uncertainty on the level 0.0005 cm^{-1}–0.001 cm^{-1}. The spectra calibration allows having the line positions with the lower uncertainty after taking into account the pressure shift. In this paper the 3200–4700 cm^{-1} region corresponding to the $\Delta P=5$ and $\Delta P=6$ series of transitions was carefully studied. Here P is a polyad number. $P=2V_1+V_2+3V_3$, where V_i ($i=1,2,3$) are harmonic oscillator quantum numbers. In the result of the multispectrum fitting the line positions and line intensities were determined. The uncertainty of the line positions measurement is 0.0003 cm^{-1} for the unblended and not very weak lines. In this work, a number of new bands were assigned and the line positions measured for the $^{16}O^{12}C^{17}O$ and $^{17}O^{12}C^{17}O$ isotopologues were used, together with those collected from the literature, to fit the effective Hamiltonian parameters for these isotopologues. The retrieved line intensities were used to fit the effective dipole moment parameters for the $\Delta P=5$ and $\Delta P=6$ series of transitions in $^{16}O^{12}C^{17}O$, $^{12}C^{17}O_2$ and $^{16}O^{12}C^{18}O$ isotopologues of carbon dioxide.

2. Experiment

Line parameters in the 3200–4700 cm^{-1} region have been retrieved from the spectra recorded in LADIR (Paris, France) [1] using enriched 17 and 18 oxygen carbon dioxide. For the readers' convenience we recall briefly the experiment performed in LADIR. Thirteen spectra were recorded at room temperature by the rapid scan interferometer Bruker IFS 125 h with unapodized resolution of 0.0056 cm^{-1} and using a metal multipass White-type cell (1-m base length). The whole optical path was under vacuum and the multipass cell was aligned to provide absorption path lengths between 4.15 and 20.15 m. The temperature inside the cell was stable to ± 0.3 K during the recording. The detailed description of the experiment is presented in our recently published paper [1]. The experimental conditions of the spectra recordings are gathered in Table 1 of the above cited paper. The main aim of that paper was the studying of the sample composition. The obtained concentrations of the carbon dioxide isotopologues in the sample are presented in Table 2 of the

Table 1
Summary of the studied bands.

Isotopologue	Number of observed bands	Number observed lines	Number of newly observed bands	Number of newly observed lines
$^{16}O^{12}C^{16}O$	19	1008	–	–
$^{16}O^{13}C^{16}O$	4	203	–	–
$^{16}O^{12}C^{18}O$	17	1571	2	37
$^{16}O^{12}C^{17}O$	29	2417	15	402
$^{16}O^{13}C^{18}O$	5	382	–	–
$^{16}O^{13}C^{17}O$	8	608	4	176
$^{18}O^{12}C^{18}O$	11	488	–	–
$^{17}O^{12}C^{18}O$	21	1680	12	553
$^{18}O^{13}C^{18}O$	3	142	–	–
$^{17}O^{12}C^{17}O$	21	1792	13	597
$^{17}O^{13}C^{18}O$	6	480	3	115
$^{17}O^{13}C^{17}O$	7	547	4	156
Total	151	11318	53	2036

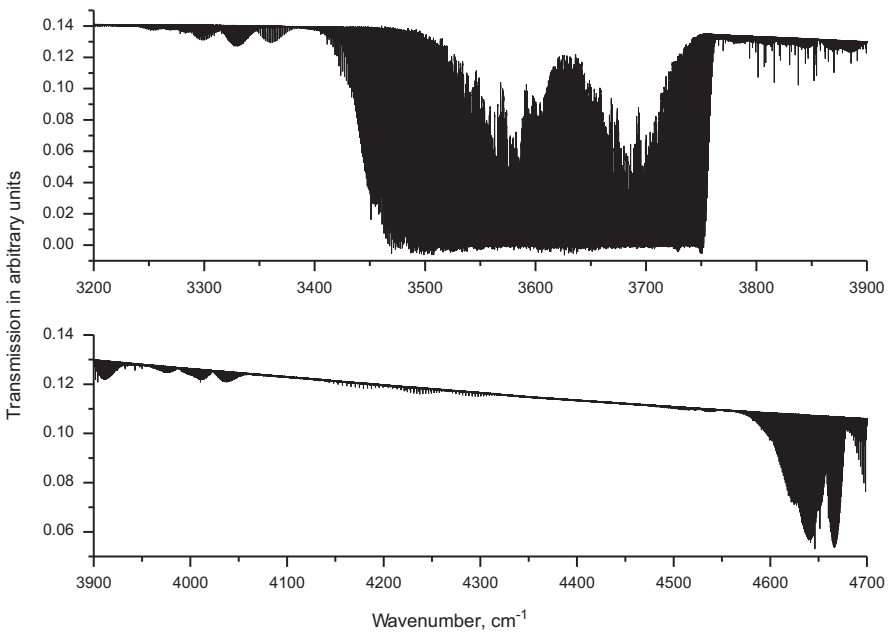

Fig. 1. Overview spectrum in the 3200–4700 cm^{-1} region of the carbon dioxide sample described in Ref. [1]: $P=31.42$ Torr, $L=2015$ cm, $T=297.7$ K.