

Line strengths of $^{16}\text{O}^{13}\text{C}^{16}\text{O}$, $^{16}\text{O}^{13}\text{C}^{18}\text{O}$, $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ and $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ between 2200 and 6800 cm^{-1}

R.A. Toth^{a,*}, C.E. Miller^a, L.R. Brown^a, V. Malathy Devi^b, D. Chris Benner^b

^a Jet Propulsion Laboratory, California Institute of Technology, MS 183-301, 4800 Oak Grove Drive, Pasadena, CA 91109, USA

^b The College of William and Mary, Department of Physics, Box 8795, Williamsburg, VA 23187-8795, USA

Received 15 November 2007; in revised form 12 December 2007

Available online 26 January 2008

Abstract

Line positions and strengths of $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ (636), $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ (638) and $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ (637), and $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ (838) bands were measured using natural and ^{13}C - and ^{18}O -enriched samples of CO_2 at room temperature. Twenty-five near infrared (NIR) absorption spectra were recorded at 0.01–0.013 cm^{-1} resolution with the McMath–Pierce Fourier transform spectrometer located at the National Solar Observatory on Kitt Peak, Arizona. Absorption cells with optical path lengths ranging from 0.347 m to 385 m were used with pressures ranging between 0.5 and 147 torr. Line strengths were obtained for 17 bands of (636) between 4697 and 6797 cm^{-1} , 13 bands of (638) between 2192 and 4954 cm^{-1} , 4 bands of (637) between 3437 and 4981 cm^{-1} and 7 bands of (838) between 2182 and 4888 cm^{-1} . Band strengths and Herman–Wallis-like F -factor coefficients were determined from least-squares fits to over 2000 measured transition intensities involving 41 different bands. The observed line positions of several bands were analyzed to obtain the upper state term values and rotational constants. Five of the $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ bands and two of the $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ bands were modeled for the first time.

© 2008 Elsevier Inc. All rights reserved.

Keywords: Carbon dioxide; Isotopes; Line positions; Intensities; Near-infrared; Enriched samples

1. Introduction

Our recent analyses [1–9] of near infrared (NIR) laboratory spectra of carbon dioxide are intended to support atmospheric remote sensing of the terrestrial planets (Earth, Mars and Venus). For this, we have already reported accurate line positions, intensities and broadening coefficients of four isotopologues involving ^{12}C - and ^{18}O -enriched CO_2 . The results for the 4500–7000 cm^{-1} have been collected into a comprehensive compilation [5] that includes parameters for nine different isotopologues. The present paper completes our comprehensive NIR study by obtaining line positions and line strengths for four ^{13}C -enriched isotopologues: $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ (636), $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ (638) and $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ (637), and $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ (838) from 2200 to 6820 cm^{-1} .

Previously, Miller et al. [8] analyzed high-resolution spectra of $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ and $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ to determine line positions and vibration–rotation parameters for 44 vibrational states (00001–10031) of (636) and 19 states (00001–00031) of (638). Several other groups examined line positions (and in some cases intensities) for the ^{13}C isotopologues as well. Teffo et al. [10] obtained spectra of ^{17}O -enriched CO_2 in the ν_2 (600–800 cm^{-1}) and ν_3 (2200–2400 cm^{-1}) regions from which frequency parameters of the 00001, 00011, and 01101 states were determined for $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ (637), $^{17}\text{O}^{13}\text{C}^{17}\text{O}$ (737) and $^{17}\text{O}^{13}\text{C}^{18}\text{O}$ (738); band strength parameters of the ν_3 band of $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ were also given. Ding et al. [11] obtained spectroscopic parameters of several vibrational states of (638) from measurements in the 4000–9500 cm^{-1} region, and Ding et al. [12] derived parameters of (637) from analysis of FTS spectra between 4000 and 8500 cm^{-1} and by CW-cavity ringdown spectroscopy (cw-CRDS) between 6130 and 6750 cm^{-1} . Wang et al. [13] recorded FTS spectra in the region of 4200–8500 cm^{-1}

* Corresponding author. Fax: +1 818 393 4445.

E-mail address: Robert.A.Toth@jpl.nasa.gov (R.A. Toth).

and obtained absolute line strengths with estimated uncertainties of $\sim 5\%$. Perevalov et al. measured line positions of (636), (637) and (638) bands obtained from ^{13}C -enriched CO_2 spectra recorded with cw-CRDS in the 5957–6122, 6745–6833 cm^{-1} [14] and 5900–7000 cm^{-1} [15] regions; however, the present study did not directly analyze any of the 17 new bands seen in [14,15].

The primary emphasis of the present study is to obtain accurate line strengths for the four ^{13}C isotopologues of CO_2 and determine band strengths and F -factor coefficients as well as vibration–rotation parameters. Some of the line positions and vibration–rotation parameters have not been previously assigned or determined; this is the case for most of the (838) bands studied here. In addition, we provide improved line positions for several bands where the existing parameters were insufficient to simulate our spectra within experimental uncertainty. We use the HITRAN 2004 compilation [16] as the standard for comparisons of line positions and line strengths. A total of 41 separate bands are considered here.

2. Experiment

All the CO_2 spectra used in the present study were recorded using the McMath–Pierce Fourier transform spectrometer (FTS) located at the National Solar Observatory on Kitt Peak. The FTS was configured with quartz halogen lamps providing the NIR source, a CaF_2 beamsplitter, and two liquid nitrogen cooled InSb detectors. The resolution was 0.01–0.013 cm^{-1} , and the integration time was 60–130 min per spectrum. The experimental conditions (sample pressures, optical path lengths, etc.) for the 25 spectra with ^{13}C - and ^{18}O -enriched CO_2 samples analyzed in this study are listed in Table 1. Spectra of natural abundance CO_2 samples were also used to obtain (636) line strengths; the experimental conditions for these can be viewed in Table 1 of Ref. [1]. Spectra were obtained at room temperature using natural samples of CO_2 and two different ^{18}O -enriched samples (94% $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ and 46% $^{16}\text{O}^{12}\text{C}^{18}\text{O}$) and 99% $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ and 95% $^{16}\text{O}^{13}\text{C}^{16}\text{O}$. Compositions of the isotopically enriched CO_2 samples were determined to $\pm 0.01\%$ through mass spectroscopic analysis by the manufacturer. The lower portion of Table 1 lists the relative isotopic abundances of the enriched CO_2 samples used in this study. The complete listing of the abundances for 9 isotopologues for the 155.xx and 166.40–166.44 runs was given previously [3]. The remaining runs, 160.xx, 165.xx, 166.21–166.24, and 152.7, are obtained using ^{13}C -enriched CO_2 samples. For the spectra obtained with the natural CO_2 sample we retrieved the standard relative abundance of $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ using intensities obtained from the enriched samples. The sample pressures were determined using three cross-calibrated Baratron capacitance manometers with 10, 100, and 1000 torr full scale ranges.

Three absorption cells were used in this study. One cell was a stainless steel multi-transversal cell with a base path length of 6 m. Sample temperatures were monitored using

three thermocouples kept in contact with the outside surface of the cell. The entire 6 m path was wrapped with insulating sheets to reduce temperature gradients along the entire cell length and stabilize the cell temperature during data acquisition. The other experiments were performed using insulated, single pass stainless steel cells 2.46 and 0.347 m long. Each of the single pass cells had four high accuracy (± 0.05 K) platinum resistance thermometer probes (Hart Scientific) inserted through the cell walls at regular intervals that provide direct contact with the gas samples. The experimental setup and data acquisition methods are similar to those given in Ref. [1].

Accurate wavenumber calibration of all the spectra was obtained using a second cell inserted into the optical beam so that well-known transitions of the 1-0 and 2-0 bands of CO [17,18] or of the $\nu_1 + \nu_3$ band of C_2H_2 [19] could be used. Observed line positions of $^{16}\text{O}^{12}\text{C}^{16}\text{O}$ [3] were also used to calibrate some spectra. The wavenumber calibration was checked using narrow H_2O lines found superimposed on top of air- or N_2 -broadened H_2O lines and originating from the small amounts of residual water vapor present in the vacuum tank enclosing the FTS; the H_2O reference line positions were taken from Toth [20]. Line positions of $^{16}\text{O}^{12}\text{C}^{16}\text{O}$ were based on low pressure runs whenever possible and corrected for self-broadened pressure shifts [2] when higher pressure spectra were used. The measured line center positions were calibrated using the multiplying factors, cv , given in Table 1, that were derived from these standards.

Survey scans of ^{18}O -enriched and ^{13}C -enriched CO_2 are shown in Fig. 1 with band and isotopologue labeling. The sample used to record the spectrum in the upper panel covering the 3400–3480 cm^{-1} region is composed mainly of $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ (47%) and $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ (33%). The P-branch of the (838) 10012 \leftarrow 00001 band is clearly seen in the 3420–3440 cm^{-1} range despite the fact that $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ constitutes only 0.3% of the total sample. The spectrum in the lower panel contains 95% ^{13}C -enriched CO_2 and shows the prominent $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ and $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ bands. Features due to residual H_2O are observed beyond 5100 cm^{-1} .

The survey spectra in Fig. 2 were obtained with 50.2 torr of 99% $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ and an optical path of 2.42 m. The upper panel covers the Fermi triad bands for those originating from the ground state and associated hot bands. The lower spectrum covers three of the Fermi tetrad bands from 6000 to 6600 cm^{-1} and includes the C_2H_2 transitions near 6500 cm^{-1} used for wavenumber calibration. The weak 30014 \leftarrow 00001 band centered at 5951 cm^{-1} is not included in the figure.

3. Data retrieval

Line positions and strengths were determined by matching the observed and synthetic spectra using the same technique applied in our previous studies [1–3]. A Voigt profile was used for the molecular line shape, and a sinc function with correction for an 8 mm aperture was assumed for the

Download English Version:

<https://daneshyari.com/en/article/5415546>

Download Persian Version:

<https://daneshyari.com/article/5415546>

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