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## The 1- $\mu\text{m}$ $\text{CO}_2$ bands and the $\text{O}_2$ (0–1) $X^3\Sigma_g^- - a^1\Delta_g$ and (1–0) $X^3\Sigma_g^- - b^1\Sigma_g^+$ bands in the Earth atmosphere

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### Abstract

The  $\text{CO}_2$  triad of bands in the 9300–9700  $\text{cm}^{-1}$  region have been observed in near infrared 0.05  $\text{cm}^{-1}$  resolution ground-based solar absorption spectra. This interval is a portion of spectra taken in the 9000–12,000  $\text{cm}^{-1}$  region, at large solar zenith angles. Considering the available line positions and pressure line shifts for  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and  $\text{O}_2$  in this region as of 2000, it was concluded that these observations show significant inconsistencies among the line positions of the species as listed in the atmospheric spectroscopy databases. The spectra allow a better definition of the  $\text{O}_2$  (0–1)  $X^3\Sigma_g^- - a^1\Delta_g$  band, with the discrete (0–1) transitions observable in the 9300–9450  $\text{cm}^{-1}$ , superimposed on a collision-induced continuum covering the 9200–9700  $\text{cm}^{-1}$  region. This continuum, as well as the (0–0) continuum in the 7900  $\text{cm}^{-1}$  region, have been previously studied only from atmospheric spectra with much lower spectral resolution. The discrete  $\text{O}_2$  (1–0) transitions of the  $X^3\Sigma_g^- - b^1\Sigma_g^+$  atmospheric B-band are observed in the 11,500–11,600  $\text{cm}^{-1}$  region, but no evidence is found for an underlying continuum. A recent laboratory study of the  $2\nu_1 + 3\nu_3$   $^{12}\text{CO}_2$  triad significantly improves the consistency between the  $\text{O}_2$ ,  $\text{H}_2\text{O}$  and  $\text{CO}_2$  lines in the atmospheric spectra.

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## 1. Introduction

The 1- $\mu\text{m}$  region is a traditional window for atmospheric remote sensing and it is used in many current and planned atmospheric remote-sensing experiments. Accurate spectroscopic parameters for the atmospheric species are essential for the analysis of data from such experiments. In particular, the improvement of the  $\text{CO}_2$  line parameters listed in the spectroscopic databases [1,2] for this region continues to be of central interest to atmospheric spectroscopy. It has been reported [3,4] that most of the tabulated  $\text{CO}_2$  levels above  $7065\text{ cm}^{-1}$  and thus the line positions, originate from DND calculations or from the spectroscopic constants derived from analysis of Venus spectra [5]. With the exception of the  $\nu_3 \Delta v = 1$  sequences, where accurate energy levels are available [6] up to the level  $(0\ 0^{\circ}12\ 1)$  [ $\nu_3 = 12$ ], it has been estimated the accuracy in the energy levels is not better than  $0.01\text{ cm}^{-1}$ . The work by Wattson et al. [7], on new high-resolution long-path  $\text{CO}_2$  laboratory spectra in this region, was aimed toward new analysis of these bands, but lacked reference line positions for calibration. The work on the CO (0–3) line positions [8–10] (not observed in atmospheric spectra), provided CO references for improved laboratory  $\text{CO}_2$  line positions in the region of interest. Recent measurements of intensities and broadening parameters for the CO (0–3) band are also available [11,12].

During March 2000, high resolution ( $0.05\text{ cm}^{-1}$ ) ground-based solar absorption spectra were obtained in the  $9000\text{--}12,000\text{ cm}^{-1}$  region, with a signal to noise ratio exceeding 300. Subsequently, we have studied these spectra for collective features of  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  as described by Goldman et al. [13].

The spectra were acquired using a Bruker 120M Fourier transform spectrometer located at the Southern Great Plains (SGP) Cloud and Radiation Testbed (CART) [14] near Lamont, Oklahoma (altitude 318 m, latitude  $36.6^{\circ}\text{N}$ , longitude  $96.5^{\circ}\text{W}$ ). The facility is part of the DOE Atmospheric Radiation Measurement (ARM) Program. The spectrometer is maintained by the University of Denver and was configured for near infrared observations during March of 2000. The instrument was equipped with a  $\text{CaF}_2$  beamsplitter, a Si diode detector and appropriate digital and optical bandpass filters for these measurements.

## 2. Results and discussion

Some of the spectra were obtained with large solar zenith angles, which show  $\text{CO}_2$  absorption lines from the 1- $\mu\text{m}$  bands in the  $9300\text{--}9700\text{ cm}^{-1}$   $2\nu_1 + 3\nu_3$  triad,  $(v'' - v') = (00001 - 20033)$ ,  $(00001 - 20032)$ , and  $(00001 - 20031)$  in HITRAN notation, with band centers at  $9388.994$ ,  $9516.969$  and  $9631.353\text{ cm}^{-1}$ , respectively. The HITRAN line positions for these bands were generated [3] with updated ground state constants, but the upper-state constants are from Ref. [5]. While the HITRAN line positions agree with the original Mandin [5] lines to within  $0.005\text{ cm}^{-1}$ , the absolute line-position accuracy was not expected to be better than  $0.01\text{ cm}^{-1}$ .

The  $\text{H}_2\text{O}$  line absorptions observed in these spectra were measured and partially analyzed in high resolution laboratory spectra [15–17]. The line positions accuracy for many of these lines is better than  $0.002\text{ cm}^{-1}$ . The numerous solar lines have been identified and studied over many years [18].

Figs. 1–4 describe the observations in several spectral intervals of the spectra (see legends under figures). In the  $9300\text{--}9450\text{ cm}^{-1}$  region ( $1.06\ \mu\text{m}$ ), the low sun spectra show discrete (0–1)  $\text{O}_2$

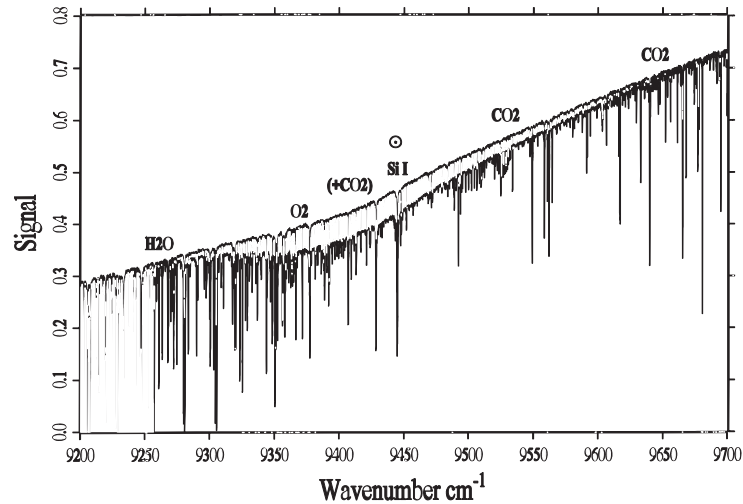


Fig. 1. The 9200–9700  $\text{cm}^{-1}$  region from ground-based solar absorption spectra obtained at high sun (solar zenith angle of  $Z = 58.9^\circ$ ) and low sun ( $Z = 79.1^\circ$ ). The spectra were recorded during the morning of March 5, 2000 at the Oklahoma SGP ARM site with a Bruker 120M FTS interferometer at  $0.05 \text{ cm}^{-1}$  resolution and each represents a coadding of four individual scans. In addition to the strong solar atomic lines and atmospheric  $\text{H}_2\text{O}$  lines, the spectra also show weaker atmospheric absorptions from several bands of interest: (1) the discrete  $(0-1) X^3\Sigma_g^- - a^1\Delta_g$   $\text{O}_2$  lines in the 9300–9450  $\text{cm}^{-1}$  superimposed on the  $\text{O}_2$  continuum; (2) the  $\text{CO}_2$  Venus 1- $\mu\text{m}$  bands in this region,  $(v'' - v') = (00001 - 20033)$ ,  $(00001 - 20032)$ , and  $(00001 - 20031)$  centered around 9389, 9517, and 9631  $\text{cm}^{-1}$ , respectively. The collision induced  $\text{O}_2X^3\Sigma_g^- - a^1\Delta_g$  continuum extends over the complete 9200–9700  $\text{cm}^{-1}$  region.

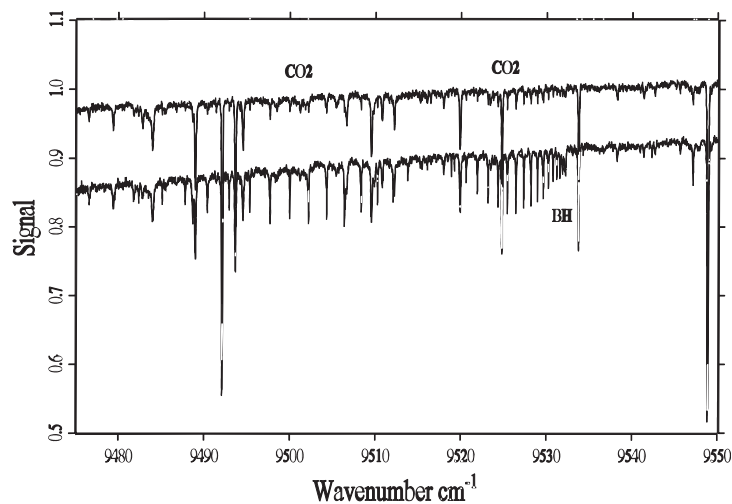


Fig. 2. The 9475–9550  $\text{cm}^{-1}$  region from Fig. 1, expanded to show the  $\text{CO}_2$  band  $(00001-20032)$ , centered at 9516.9  $\text{cm}^{-1}$ . The band head (BH) is at 9532.1  $\text{cm}^{-1}$ .

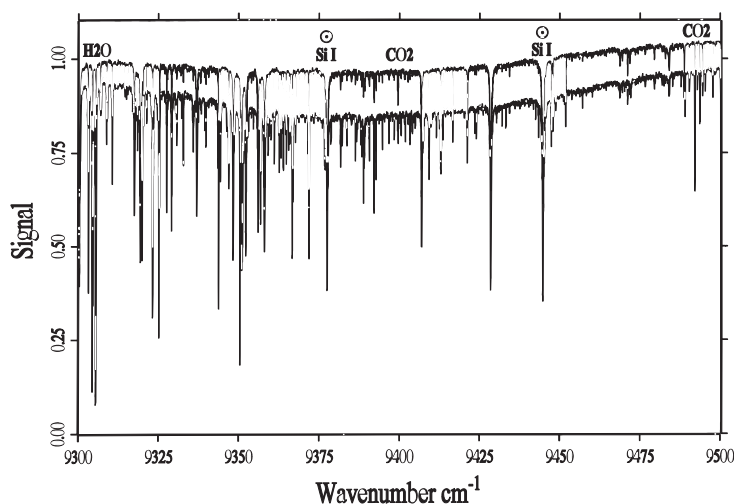


Fig. 3. The 9300–9500  $\text{cm}^{-1}$  region from Fig. 1, expanded to show the discrete  $\text{O}_2$  (0–1) transitions of the  $X^3\Sigma_g^- - a^1\Delta_g$  band, centered at 9365.9  $\text{cm}^{-1}$ , and the  $\text{CO}_2$  (0 0 0 0 1–2 0 0 3 3) band centered at 9389.0  $\text{cm}^{-1}$ . Also shown is part of the  $P$ -branch of the  $\text{CO}_2$  (0 0 0 0 1–2 0 0 3 2) band centered at 9516.9  $\text{cm}^{-1}$ .

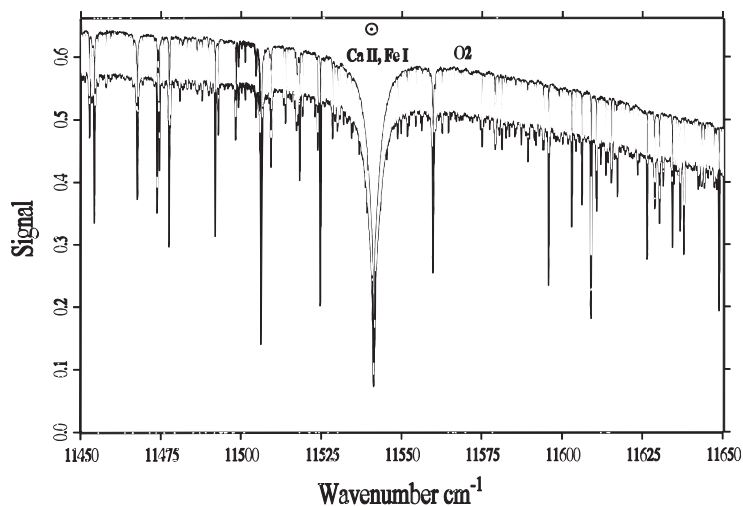


Fig. 4. The 11,450–11,650  $\text{cm}^{-1}$  region from the same two spectra used in Fig. 1. These two scans are displaced for clarity. This region shows many discrete  $\text{O}_2$  (1–0) transitions of the  $X^3\Sigma_g^- - b^1\Sigma_g^+$  band, centered at 11,565  $\text{cm}^{-1}$ , with no underlying continuum.

transitions of the  $X^3\Sigma_g^- - a^1\Delta_g$  band, superimposed on a collision-induced continuum extending from 9200 to 9700  $\text{cm}^{-1}$ . This continuum, as well as the stronger (0–0)  $X^3\Sigma_g^- - a^1\Delta_g$  continuum (and discrete lines) in the 7700–8100  $\text{cm}^{-1}$  region (1.27  $\mu\text{m}$ ) have recently gained renewed interest from studies of atmospheric spectra at much lower resolution [19–21], and motivated new laboratory and field studies [22–26]. The estimated accuracy of the discrete line positions is 0.001  $\text{cm}^{-1}$ .

Table 1  
Typical measured values of H<sub>2</sub>O line-shift (in cm<sup>-1</sup> atm<sup>-1</sup>)

Band	Ref.	Self	[Air]	[N <sub>2</sub> ]	[O <sub>2</sub> ]
(000 – 221), (000 – 301) 0.72 μm > 100 lines, 304 K, 383 K	[33]				
Average value for 296 K		—	–0.0166	–0.0133	–0.0261
Max.			–0.0295	–0.0272	–0.0355

Updated line intensities for the 1.27-μm band have been recently calculated at the University of Denver, based on techniques introduced in previous studies by Goldman et al. [27], which properly take into account mixing-of-state effects. These intensities give improved agreement, over the HITRAN 2001 [28] lines, with both laboratory [22] and atmospheric [26] data.

In the 11,500–11,600 cm<sup>-1</sup> region (0.86 μm), the discrete transitions of the O<sub>2</sub> (1–0) X<sup>3</sup>Σ<sub>g</sub><sup>-</sup> – b<sup>1</sup>Σ<sub>g</sub><sup>+</sup> atmospheric B-band are observed, with absorptions similar in magnitude to those in the 1.06-μm band, but with no underlying continuum. Consistent with this result, this band is not observable in laboratory path spectra in which the weak line structure is further smeared out by lower resolution or by pressure broadening [23,29]. As summarized by Gamache et al. [20], the molecular constants used for the HITRAN line listing are from Albritton et al. [30] (this is a correction to reference no. 43 given in Gamache et al. [20]) and from Rouillé et al. [31] for the b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>(*v* = 0) and X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>(*v* = 1), respectively. The accuracy in the line positions can be estimated as 0.005 cm<sup>-1</sup>.

In principle, the solar absorption spectra described above could be accurately calibrated in wavenumber (cm<sup>-1</sup>), as the positions of observed H<sub>2</sub>O and O<sub>2</sub> lines are accurately known. Only weak and medium intensity H<sub>2</sub>O lines from Refs. [15–17] are useful for the wavenumber calibration, as the strong lines are fully absorbed. The O<sub>2</sub> and CO<sub>2</sub> line absorptions do not exceed 15% in these spectra. However, all the observed line positions include line pressure shifts, for H<sub>2</sub>O, O<sub>2</sub> and CO<sub>2</sub>. The line shifts are molecule and transition dependent, not always known to the needed accuracy, while the reference laboratory lines are provided as free from pressure shifts.

Tables 1–3 show measured results from the latest published line-shift studies of several bands of H<sub>2</sub>O [32–34], O<sub>2</sub> [35–37], and CO<sub>2</sub> [38–40]. The individual publications reveal significant disagreements among the reported experimental results. Despite these discrepancies in the line shifts, it was concluded that the CO<sub>2</sub> line positions in the Venus bands are not consistent with the more accurate positions of H<sub>2</sub>O and O<sub>2</sub>. As an example, we calibrated the 9400–9600 cm<sup>-1</sup> region by the O<sub>2</sub> shift-free reference lines in this region (from [1]), which gave O<sub>2</sub> line position consistency of ≈ 0.0008 cm<sup>-1</sup>. Applying the same calibration to all spectral lines in this region, and considering the range of the O<sub>2</sub> shifts [36], imply that the H<sub>2</sub>O lines need to be shifted by –0.015 to –0.02 cm<sup>-1</sup>, which is in the expected range [32–34]. However, for CO<sub>2</sub> we obtain implied shifts in the range of –0.02 to +0.02 cm<sup>-1</sup>, significantly out of the range of the experimental results [38–40]. Thus, the atmospheric spectra confirm the need for improvement in the CO<sub>2</sub> line positions and thus energy levels [13].

Table 2  
 Typical measured values of O<sub>2</sub> line-shift (in cm<sup>-1</sup> atm<sup>-1</sup>)

Band	Ref.	[Self]	[Air]	[N <sub>2</sub> ]
a <sup>1</sup> Δ <sub>g</sub> ( <i>v</i> = 0) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 1.27 μm 118 lines, 299 K Average shift	[35]	-0.035 ± 0.016	—	—
b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ( <i>v</i> = 0) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 0.76 μm 59 lines, 299 K Average shift	[35]	-0.011 ± 0.0025	—	—
b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ( <i>v</i> = 1) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 0.69 μm 58 lines, 299 K Average shift	[35]	-0.011 ± 0.0045	—	—
b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ( <i>v</i> = 1) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 0.69 μm 17 lines, 293 K Average shift	[37]	-0.014 ± 0.004	—	—
b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ( <i>v</i> = 2) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 0.63 μm 43 lines, 299 K Average shift	[35]	-0.038 ± 0.012	—	—
b <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> ( <i>v</i> = 0) – X <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ( <i>v</i> = 0), 0.76 μm <i>P1P1</i> – <i>R21R21</i> , 296 K Range <i>J'</i> = 0 to <i>J</i> <sub>max</sub> <i>R17R17</i>	[36]	-0.0025 → -0.0087 -0.0051(7)	— —	-0.0020 → -0.0088 —

In a recent laboratory study by Ding et al. [41], line positions for the 2*v*<sub>1</sub> + 3*v*<sub>3</sub> <sup>12</sup>CO<sub>2</sub> triad have been reported, showing a systematic shift of  $-1.33(19) \times 10^{-2}$  cm<sup>-1</sup> from Mandin's lines [5], based on acetylene lines accurate to  $2 \times 10^{-4}$  cm<sup>-1</sup>. Improved spectroscopic parameters are also provided. It is interesting to note that the new line positions practically remove the discrepancies discussed above. The atmospheric CO<sub>2</sub> line positions are now within  $\pm 0.0015$  cm<sup>-1</sup> of the laboratory positions, and do not contradict the reported line shifts [38–40]. It is planned to incorporate these results into future editions of the HITRAN database.

### 3. Conclusions

Spectral features of CO<sub>2</sub>, H<sub>2</sub>O and O<sub>2</sub> transitions in the 1-μm atmospheric window have been reviewed, considering the available atmospheric and laboratory spectra. Some inconsistencies in the database are resolved on the basis of recent laboratory data. Outstanding issues and future needs are discussed.

Table 3

Typical measured values of CO<sub>2</sub> line-shift (in cm<sup>-1</sup> atm<sup>-1</sup>)

Band	Ref.	Self	Air	N <sub>2</sub>
3ν <sub>3</sub> , 1.43 μm P,R 300 K R(6)	[38]	-0.014 ± 0.004	—	—
ν <sub>3</sub> , 4.3 μm P(40) – R(40) 294 K 34 lines, Max. P(20)	[39]	—	—	-0.00372(74) -0.00332(18)
00 <sup>0</sup> 1 – (10 <sup>0</sup> 0 – 02 <sup>0</sup> 0) <sub>II</sub> , 9.4 μm P(46) – R(44), 296 K 46 lines, Max. P(20)	[40]	—	-0.00307(26) -0.00203(11)	-0.00425(95) -0.00222(12)
00 <sup>0</sup> 1 – (10 <sup>0</sup> 0 – 02 <sup>0</sup> 0) <sub>I</sub> , 10.4 μm P(46) – R(44), 296 K 46 lines, Max. P(20)	[40]	—	-0.00432(75) -0.00204(13)	-0.00469(137) -0.00192(15)

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