



Contents lists available at SciVerse ScienceDirect

# Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: [www.elsevier.com/locate/jqsrt](http://www.elsevier.com/locate/jqsrt)

## Infrared spectroscopy of $^{17}\text{O}$ - and $^{18}\text{O}$ -enriched carbon dioxide in the 1700–8300 $\text{cm}^{-1}$ wavenumber region

O.M. Lyulin<sup>a</sup>, E.V. Karlovets<sup>a</sup>, D. Jacquemart<sup>b,c</sup>, Y. Lu<sup>d</sup>, A.W. Liu<sup>d</sup>, V.I. Perevalov<sup>a,\*</sup><sup>a</sup> Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, Siberian Branch, Russian Academy of Science, 1 Akademian Zuev sq., 634021 Tomsk, Russia<sup>b</sup> UPMC Univ Paris 06, UMR 7075, Laboratoire de Dynamique Interactions et Réactivité, Case Courrier 49, Bât. F 74, 4 Place Jussieu, 75252 Paris Cedex 05, France<sup>c</sup> CNRS, UMR 7075, Laboratoire de Dynamique Interactions et Réactivité, Case Courrier 49, Bât. F 74, 4 Place Jussieu, 75252 Paris Cedex 05, France<sup>d</sup> Hefei National Laboratory for Physical Sciences at Microscale, Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, China

## ARTICLE INFO

## Article history:

Received 24 May 2012

Received in revised form

30 June 2012

Accepted 30 June 2012

Available online 14 July 2012

## Keywords:

Carbon dioxide

Isotopologues

Infrared

Vibration-rotation

Line positions

Spectroscopic constants

HITRAN

CDS

## ABSTRACT

The assignment of the high resolution Fourier transform spectra of carbon dioxide enriched in  $^{17}\text{O}$  and  $^{18}\text{O}$  which were recorded in LADIR (Paris, France) with the Bruker IFS 125-HR between 1800 and 9000  $\text{cm}^{-1}$  and in USTC (Hefei, China) with the Bruker IFS 120-HR between 1700 and 9000  $\text{cm}^{-1}$  was performed. In total 239 bands of 12 isotopologues:  $^{16}\text{O}^{12}\text{C}^{16}\text{O}$ ,  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ ,  $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ ,  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ ,  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ ,  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ ,  $^{17}\text{O}^{13}\text{C}^{17}\text{O}$  and  $^{17}\text{O}^{13}\text{C}^{18}\text{O}$  were observed. Among them, 99 bands were observed for the first time. The majority of new observed bands belong to  $^{17}\text{OCO}$  isotopologues. The positions of 23,003 lines were determined with the experimental uncertainty on the level of 0.001  $\text{cm}^{-1}$ . The spectroscopic constants were fitted to the observed line positions for all observed bands.

© 2012 Elsevier Ltd. All rights reserved.

## 1. Introduction

This paper is the second one from a series dedicated to near infrared spectroscopy of carbon dioxide, driven by the need for spectroscopic reference standards to support remote sensing of the planetary atmospheres of Mars, Venus and the Earth. This series is aimed mostly to extend and to improve spectral line parameters of  $^{17}\text{OCO}$  isotopologues of carbon dioxide. The information about spectral line parameters of these isotopologues contained in CDS [1–3] and HITRAN [4] databases is not complete. A considerable part of the spectral line parameters for  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  and  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologues in the wavenumber region higher than

3000  $\text{cm}^{-1}$  came to these databases from the calculations performed within the framework of the method of effective operators [5,6]. Because of the lack of the experimental spectroscopic information the sets of the effective Hamiltonian parameters used for the calculation of both line positions and intensities of these isotopologues are not complete. Some important parameters of their effective Hamiltonians are still missing. The line intensities were calculated using effective dipole moment parameters of the principal isotopologue. To get the new experimental information about the spectral line parameters of  $^{17}\text{OCO}$  isotopologues two series of experiments were performed with the  $^{17}\text{O}$  enriched samples of carbon dioxide in LADIR (Paris, France) and in USTC (Hefei, China). The first paper of this series [7] is devoted to establishing the isotopic composition of the sample used in LADIR. In addition the line intensities of several bands of different isotopologues were measured

\* Corresponding author.

E-mail address: vip@lts.iao.ru (V.I. Perevalov).

for the first time in that paper. This paper is mostly devoted to the assignment of the spectra recorded in LADIR and in USTC. We have also determined the line positions of all assigned lines and the spectroscopic constants for all assigned bands. The uncertainties of the line position determination are on the level of  $0.001 \text{ cm}^{-1}$ .

## 2. Experiment

### 2.1. LADIR

Thirteen spectra were recorded in Paris with the rapid scan interferometer Bruker IFS 125 HR of LADIR with unapodized resolution of  $0.0056 \text{ cm}^{-1}$  and by 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 cell was equipped with KCl windows. The temperature of the gas inside the cell was obtained by averaging measurements performed by four platinum probes inside the cell. The temperature inside the cell was kept stable at  $\pm 0.3 \text{ K}$  during the recording. The Bruker IFS 125 was equipped with a  $\text{CaF}_2$  beam splitter, and an InSb detector for all spectra except one spectrum for which an InGaAs detector was used to cover the  $6000\text{--}9000 \text{ cm}^{-1}$  spectral range with a better signal to noise ratio. The detailed description of the experiment and the way of retrieving the spectral line parameters are presented in our recently published paper [7]. The experimental conditions of the spectra recordings are gathered in Table 1 of the above cited paper.

The sample of carbon dioxide has been furnished by ISOTECH and gives the following Mass Spectroscopy specifications for oxygen: 41.0% of  $^{16}\text{O}$  atom, 49.02% of  $^{17}\text{O}$  atom and 9.99% of  $^{18}\text{O}$  atom. No specification concerning carbon atom has been given. The purity of the sample is given at 99.9% of  $\text{CO}_2$ .

The main effort undertaken in Ref. [7] was devoted to establishing the isotopic composition of the ISOTECH sample. It was found that six isotopologues have large abundances, approximately from 1% to 40%. So the absorption spectra of this sample are very rich.

### 2.2. USTC

The  $^{17}\text{O}$  enriched carbon dioxide sample was purchased from ICON Services. The stated isotopic concentration for the  $^{17}\text{O}$  oxygen atom is 49%. The isotope abundance was studied by a photo-ionization mass spectroscopy (PIMS) experiment. The measurements were performed with an electron time-of-flight mass spectrometer of the photochemistry end-station of National Synchrotron Radiation Laboratory (Hefei). The abundances of  $^{12}\text{C}^{17}\text{O}_2$  and  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  were determined as 27% and 39%, respectively. The accuracy of the PIMS measurement was estimated to be about 1%.

Thirteen absorption spectra were recorded in spectral range from  $1700$  to  $9000 \text{ cm}^{-1}$ , with a Bruker IFS 120HR Fourier-transform spectrometer (FTS) equipped with a path length adjustable multi-pass gas cell. The maximum optical path length is 105 m. The cell was operated at room temperature, stabilized by an air-conditioning system. The pressure was measured by the manometer (MKS Baratron 627B) with 20 Torr full-scale range and 0.15% accuracy. Different band-pass optical filters were applied to improve the signal to noise ratio. The line positions were calibrated using the absorption lines of water and  $^{12}\text{C}^{16}\text{O}_2$  given in HITRAN database [4]. The experimental conditions are presented in Table 1. The overview spectrum is presented in Fig. 1.

The line positions measured in LADIR and in USTC are in a good agreement. Majority of them coincide within  $0.001 \text{ cm}^{-1}$ . Though the similar FTS technique is used in both laboratories the USTC multipass cell enables to reach longer pathways than that of LADIR. It consequently allowed a better detection of the very weak bands as shown in Fig. 2 for the Q-branch of 11101-00001 band of  $^{17}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologue. Whereas the lines of this band are on the noise level in LADIR spectrum, these transitions in USTC spectrum are strong enough to be detected and assigned.

## 3. Spectra assignment

The assignment of the recorded spectra has been performed using the atmospheric version of the CDSD databank [1]. However, this databank does not contain

**Table 1**  
Experimental conditions (USTC).

Spectral region ( $\text{cm}^{-1}$ )	Pressure (Torr)	Path length (m)	Resolution ( $\text{cm}^{-1}$ )	Light source	Beam splitter	Detector	Sample scans
1700–2100	6.7	15	0.004	Globar	KBr	InSb	324
1700–2100	6.7	69	0.004	Globar	KBr	InSb	324
2000–2400	6.7	15	0.004	Globar	KBr	InSb	378
2000–2400	6.7	69	0.004	Globar	KBr	InSb	702
2550–3250	6.7	15	0.005	Tungsten	KBr	InSb	408
2550–3250	6.7	69	0.005	Tungsten	KBr	InSb	408
3300–4300	6.7	15	0.006	Tungsten	$\text{CaF}_2$	InSb	648
3300–4300	6.7	87	0.006	Tungsten	$\text{CaF}_2$	InSb	729
4100–5000	6.7	15	0.008	Tungsten	$\text{CaF}_2$	InSb	535
4100–5000	7.0	87	0.008	Tungsten	$\text{CaF}_2$	InSb	749
5000–6300	6.7	15	0.01	Tungsten	$\text{CaF}_2$	InSb	798
5000–6300	7.0	87	0.01	Tungsten	$\text{CaF}_2$	InSb	931
5500–9000	6.3	105	0.015	Tungsten	$\text{CaF}_2$	Ge	1188

spectral line parameters for the  $^{12}\text{C}^{17}\text{O}_2$ ,  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $^{13}\text{C}^{17}\text{O}_2$ ,  $^{17}\text{O}^{13}\text{C}^{18}\text{O}$  and  $^{13}\text{C}^{18}\text{O}_2$  isotopologues of carbon dioxide, while these species have large or nonnegligible abundances in the studied samples. To provide the assignment process with the reference spectral line parameters of the above listed isotopologues the positions and intensities of the lines were calculated using the effective Hamiltonian parameters published by Chedin [8], Chedin and Teffo [9] and the effective dipole moment parameters of the principal isotopologue adopted for the generation of the atmospheric version of CDS database [1]. In both LADIR and USTC spectra, CO and OCS weak transitions

have been observed. These molecules were found as impurities coming from the commercial samples of gas.  $\text{H}_2\text{O}$  lines were also observed in the LADIR and USTC spectra. Finally weak  $\text{N}_2\text{O}$  transitions were detected in USTC spectra coming from a previous study on this gas. The assignments of the lines of these gases were performed with the help of the HITRAN database [4].

A summary of the observed bands of  $\text{CO}_2$  is presented in Table 2. In Fig. 3 a small fragment of the one of the observed spectra is presented with the assignments of the isotopologues to which the lines belong. One can see from this figure that the spectrum is very complicated because of the contributions from a large number of isotopologues.

The observed line positions together with their assignments are given in the Supplementary materials. The estimated accuracy of these line positions is better than  $0.001\text{ cm}^{-1}$ . Although the calibration performed for LADIR spectra [7] allows having the accuracy of the line positions on the level of  $0.0001\text{ cm}^{-1}$  we did not reach this accuracy because we did not take into account the pressure shift of the line positions. This will be done in the next papers devoted to the retrieval of the spectral line parameters.

#### 4. Band-by-band rotational analysis

In the case of unperturbed bands, the rotational analysis could be performed using the standard equation for the vibration–rotation energy levels:

$$F_v(J) = G_v + B_v J(J+1) - D_v J^2(J+1)^2 + H_v J^3(J+1)^3 \quad (1)$$

where  $G_v$  is the vibrational term value,  $B_v$  is the rotational constant,  $D_v$  and  $H_v$  are centrifugal distortion constants.

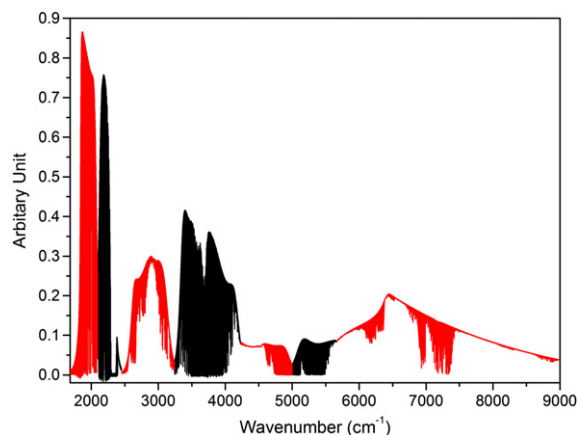


Fig. 1. The overview of transmission spectrum recorded at USTC. Alternation of the colors is chosen to separate different spectral regions corresponding to Table 1.

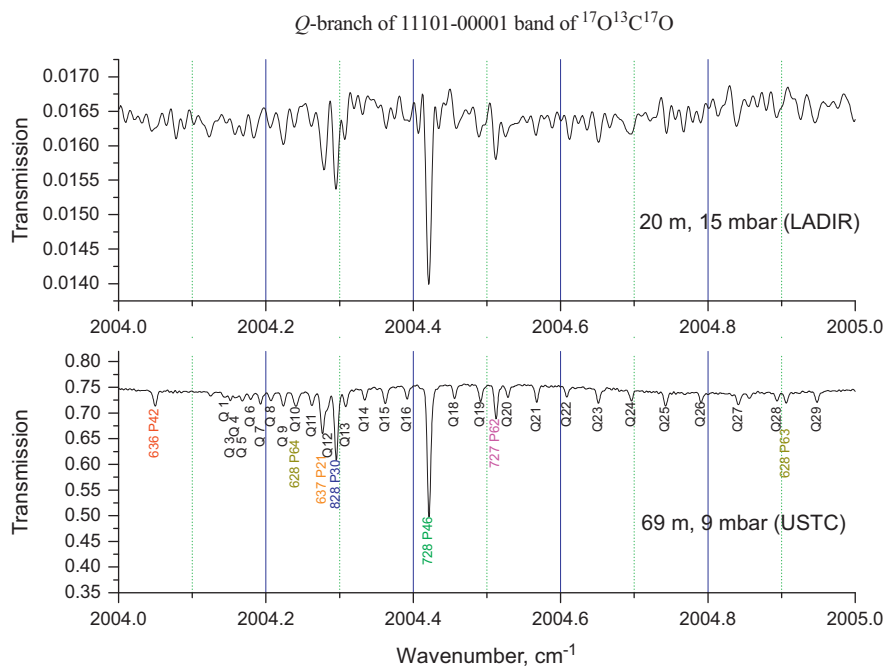


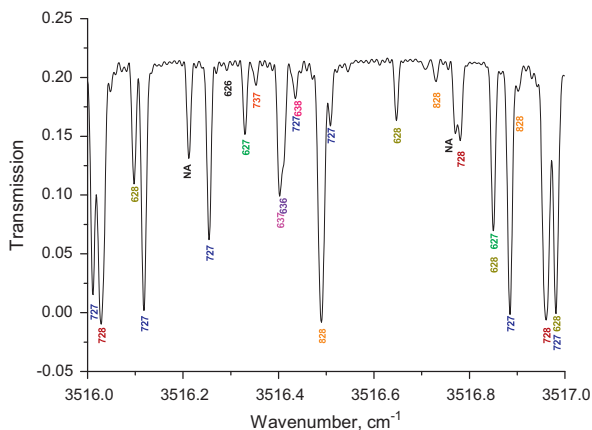
Fig. 2. Q-branch of 11101-00001 band of  $^{17}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologue (transmission spectra in arbitrary units). Upper panel: LADIR spectrum ( $L=20\text{ m}$ ,  $P=15\text{ mbar}$ ). Lower panel: USTC spectrum ( $L=69\text{ m}$ ,  $P=9\text{ mbar}$ ). HITRAN notations for the isotopologues are used 636— $^{16}\text{O}^{13}\text{C}^{16}\text{O}$ , 628— $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ , 637— $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ , 828— $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ , 728— $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  and 727— $^{17}\text{O}^{12}\text{C}^{17}\text{O}$ .

The spectroscopic parameters were fitted directly to the observed wavenumbers. In the case of the vibrational levels having e and f sublevels the spectroscopic constants

**Table 2**

Summary of the assigned bands.

Isotopologue	Number of observed bands	Number of newly observed bands
$^{16}\text{O}^{12}\text{C}^{16}\text{O}$	37	0
$^{16}\text{O}^{12}\text{C}^{17}\text{O}$	50	31
$^{17}\text{O}^{12}\text{C}^{17}\text{O}$	35	32
$^{17}\text{O}^{12}\text{C}^{18}\text{O}$	29	18
$^{16}\text{O}^{12}\text{C}^{18}\text{O}$	33	0
$^{18}\text{O}^{12}\text{C}^{18}\text{O}$	16	2
$^{16}\text{O}^{13}\text{C}^{16}\text{O}$	8	0
$^{16}\text{O}^{13}\text{C}^{17}\text{O}$	8	3
$^{17}\text{O}^{13}\text{C}^{17}\text{O}$	8	7
$^{17}\text{O}^{13}\text{C}^{18}\text{O}$	6	5
$^{16}\text{O}^{13}\text{C}^{18}\text{O}$	5	0
$^{18}\text{O}^{13}\text{C}^{18}\text{O}$	4	1
Total	239	99



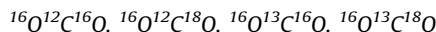
**Fig. 3.** Fragment of the spectra of carbon dioxide enriched by  $^{17}\text{O}$  and  $^{18}\text{O}$ . Twenty four lines are assigned to ten isotopologues:  $626\text{--}^{16}\text{O}^{12}\text{C}^{16}\text{O}$ ,  $628\text{--}^{16}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $727\text{--}^{17}\text{O}^{12}\text{C}^{17}\text{O}$ ,  $627\text{--}^{16}\text{O}^{12}\text{C}^{17}\text{O}$ ,  $728\text{--}^{17}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $636\text{--}^{16}\text{O}^{13}\text{C}^{16}\text{O}$ ,  $637\text{--}^{16}\text{O}^{13}\text{C}^{17}\text{O}$ ,  $638\text{--}^{16}\text{O}^{13}\text{C}^{18}\text{O}$  and  $828\text{--}^{18}\text{O}^{12}\text{C}^{18}\text{O}$ . NA means that line is not assigned. Note that the negative transmission appeared in this figure due to the effect of the apparatus function.

**Table 3**Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the 11101 and 11102 vibrational states of  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$  and for the 11112 vibrational state of  $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ .

State ( $V_1 V_2 I_2 V_3 r \epsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	Fitted bands	$\Delta G_v^a$	Observed lines <sup>b</sup>	$n/N^c$
<b><math>^{18}\text{O}^{12}\text{C}^{18}\text{O}</math></b>							
11102f	1868.7035(4) <sup>d</sup>	0.347674(3)	0.123(5)	11102f-00001e	1868.7035(4)	Q24	8/8
11102e	1868.7045(3)	0.3470028(7)	0.1150(4)	11102e-00001e	1868.7045(3)	P42	15/15
11101e	2024.5271(2)	0.3474623(3)	0.09964(9)	11101e-00001e	2024.5271(2)	P56	21/26
11101f	2024.5283(3)	0.348290(2)	0.097(2)	11101f-00001e	2024.5283(3)	Q34	9/15
<b><math>^{18}\text{O}^{13}\text{C}^{18}\text{O}</math></b>							
11112e	4056.4126(2)	0.344641(3)	0.112(1)	11112e-01101e	3417.9470(2)	P41/R17	25/25
11112f	4056.4129(2)	0.345379(3)	0.119(2)	11112f-01101f	3417.9473(2)	P42/R20	27/27

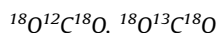
<sup>a</sup>  $\Delta G_v = G'_v - G''_v$ .<sup>b</sup> Observed branch with the maximum value of the total angular momentum quantum number.<sup>c</sup>  $N$  is the number of the observed lines and  $n$  is the number of the lines included in the fit.<sup>d</sup> Between parentheses, the confidence intervals are 1 SD in units of the last quoted digit.

for these sublevels were considered independently. The lower state rotational constants were constrained to their literature values. In the cases when a given vibrational level was reached by several transitions the line positions of all respective bands were fitted simultaneously.

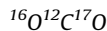


As it follows from Table 2 all assigned bands for these isotopologues were already studied in the literature. But nevertheless we have determined the respective spectroscopic constants using our line positions. The lower state constants were constrained to the values published in Ref. [10]. The determined constants are presented in the Supplementary materials.

It should be emphasised that 01111-00001 band of  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  was observed before only in Venus [11] and Mars [12] spectra and the 21101-01101 band of the same isotopologue was observed before only in Venus spectra [13].



16 bands of  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$  and 4 bands of  $^{18}\text{O}^{13}\text{C}^{18}\text{O}$  isotopologues of carbon dioxide in LADIR and USTC spectra were identified. Two bands of  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$ , namely, 11101-00001 and 11102-00001 and one band 11112-01101 of  $^{18}\text{O}^{13}\text{C}^{18}\text{O}$  were observed for the first time. The spectroscopic constants for these bands are presented in Table 3. The spectroscopic constants for other bands are given in the Supplementary materials. To fit the spectroscopic parameters of the upper states of these bands the spectroscopic parameters of the lower states were taken from Ref. [10] for  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$  and from Ref. [14] for  $^{18}\text{O}^{13}\text{C}^{18}\text{O}$ .



The enrichment of both LADIR and USTC samples with  $^{17}\text{O}$  oxygen is very high (about 50%). Because of this a lot of bands of  $^{17}\text{O}\text{CO}$  isotopologues of carbon dioxide were identified in both LADIR and USTC spectra. In total 50 bands of  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  isotopologue were identified in these spectra and 31 of them were observed for the first time. In Table 4 our spectroscopic constants for all observed bands are presented. In this table are also given the

**Table 4**  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed bands of  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  in this work.

State ( $V_1 V_2 I_2 V_3 r \epsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	$n_{\text{rot}}/N_{\text{tot}}^a$	Fitted bands	$\Delta G_v^b$	Observed lines <sup>c</sup>	$n/N^d$	RMS <sup>e</sup>	Notes <sup>f</sup>
11102f	1916.6921(1) <sup>§</sup>	0.3799022(2)	0.14634(9)		48/51	11102f-00001e 11102f-00001e	1916.6921(1) 1916.70	Q52 Q24	48/51 8	0.38	Ref. [16]
11102e	1916.69237(7)	0.3790373(1)	0.13975(3)		105/108	11102e-00001e 11102e-00001e	1916.69237(7) 1916.70	P60/R59 P40	105/108 9	0.38	Ref. [16]
11101f	2062.0984(1)	0.3798438(2)	0.11411(8)		50/53	11101f-00001e 11101f-00001e	2062.0984(1) 2062.10	Q53 Q31	50/53 5	0.34	Ref. [17]
11101e	2062.09862(6)	0.37894026(8)	0.11784(2)		111/115	11101e-00001e 11101e-00001e	2062.09862(6) 2062.10	P71/R56 P51/R14	111/115 24	0.34	Ref. [17]
00011e	2340.01320(5)	0.37563039(4)	0.125140(5)		169/182	00011e-00001e	2340.01320(5)	P90/R97	169/182	0.28	
00011e	2340.013299(11)	0.375630369(45)	0.125150(18)	0.004(1)	96	00011e-00001e	2340.013299(11)	P72/R75	96		Ref. [15]
00011e	2340.013299(11)	0.375630392(36)	0.125154(15)	0.004(1)	59	00011e-10001e		P49/R45	59		Ref. [18]
00011e	2340.013299(11)	0.375630392(36)	0.125154(15)	0.004(1)	63	00011e-10002e		P48/R51	63		Ref. [18]
00011e	2340.01360(17)	0.37563509(237)	0.13507(331)	4.9(14)		00011e-00001e	2340.01360(17)				Ref. [19]
20003e	2524.24798(8)	0.3792052(3)	0.1689(3)	0.36(6)	103/107	20003e-00001e 20003e-00001e	2524.24798(8) 2524.25	P51/R56 P40/R38	103/107 67	0.23	Ref. [20]
20002e	2641.24021(7)	0.3780471(2)	0.1206(1)	0.42(3)	119/119	20002e-00001e 20002e-00001e	2641.24021(7) 2641.24	P55/R63 P42/R44	119/119 69	0.17	Ref. [20]
12201e	2743.4008(1)	0.3800315(2)	0.13887(7)		49/53	12201e-01101e	2078.6718(1)	P57	49/53	0.34	
12201f	2743.4014(1)	0.3800280(2)	0.12003(8)		42/53	12201f-01101f	2078.6724(1)	P56	42/53	0.34	
20001e	2775.59222(6)	0.3792655(2)	0.0922(2)	0.50(5)	193/202	20001e-01101e 20001e-01101f 20001e-00001e 20001e-01101e	2110.86318(6) 2110.86318(6) 2775.59222(6) 2110.70	P57/R8 Q48 P52/R53 P32	53/58 37/38 103/106 3	0.21 0.21 0.23	Ref. [21]
01111e	2992.30224(5)	0.37607852(6)	0.12686(1)		160/215	01111e-01101e 01111e-01101f 01111e-00001e	2327.57320(5) 2327.57320(5) 2992.30224(5)	P81/R78 Q7 P38/R27	109/147 3/6 48/62	0.41 0.41 0.56	
01111e	2992.299674(27)	0.376078292(77)	0.126788(46)	-0.010(7)		01111e-01101e		P63/R66	61		Ref. [15]
01111f	2992.30232(6)	0.37664410(6)	0.12772(1)		134/193	01111f-01101f 01111f-01101e 01111f-00001e	2327.57328(6) 2327.57328(6) 2992.30232(6)	P81/R78 Q8 Q43	103/145 2/7 29/41	0.41 0.41 0.56	
01111f	2992.299674(27)	0.376643978(77)	0.127662(46)	-0.007(7)		01111f-01101f		P63/R66	59		Ref. [15]
21103e	3153.7281(1)	0.3792309(2)	0.15288(8)		72/87	21103e-00001e	3153.7281(1)	P53/R53	72/87	0.45	
21102f	3308.7530(2)	0.3795818(6)	0.1287(3)		24/30	21102f-00001e	3308.7530(2)	Q43	24/30	0.3	
21102e	3308.75391(9)	0.3784990(1)	0.12701(4)		96/104	21102e-00001e	3308.75391(9)	P61/R57	96/104	0.3	
21101f	3475.6286(1)	0.3803171(4)	0.1036(3)		58/66	21101f-01101f	2810.8996(1)	P35/R39	58/66	0.43	
21101e	3475.6289(1)	0.3790123(4)	0.1106(3)		64/69	21101e-01101e 10012e-10001e	2810.8999(1) 2215.24222(5)	P36/R39 P31	64/69 19/21	0.43 0.26	
10012e	3591.26955(5)	0.3758084(1)	0.14700(7)	0.19(1)	216/253	10012e-10002e 10012e-00001e	2318.98308(5) 3591.26955(5)	P64/R56 P64/R73	71/101 126/131	0.45 0.19	
02211f	3645.00074(9)	0.3770868(2)	0.12914(5)		67/98	02211f-02201f	2315.15268(9)	P64/R58	67/98	0.41	
02211e	3645.00084(9)	0.3770864(2)	0.13078(5)		71/98	02211e-02201e 10011e-10001e	2315.15278(9) 2317.32899(5)	P64/R58 P66/R53	71/98 62/88	0.41 0.49	

Table 4 (continued)

State ( $V_1 V_2 I_2 V_3 r \epsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	$n_{tot}/N_{tot}^a$	Fitted bands	$\Delta G_v^b$	Observed lines <sup>c</sup>	$n/N^d$	RMS <sup>e</sup>	Notes <sup>f</sup>
10011e	3693.35632(5)	0.3757491(1)	0.10682(9)	0.12(2)	270/303	10011e-10002e 10011e-00001e	2421.06985(5) 3693.35632(5)	P41/R45 P68/R63	79/84 129/131	0.37 0.19	
30003e	3898.24561(8)	0.3778114(2)	0.1491(1)		82/83	30003e-00001e	3898.24561(8)	P42/R44	82/83	0.26	
30002e	4023.41838(9)	0.3783518(3)	0.0912(2)		77/83	30002e-00001e	4023.41838(9)	P42/R42	77/83	0.32	
30002e	4023.4187(33)	0.378357(20)	0.1029(27)			30002e-00001e	4023.4187(33)				Ref. [22]
11112f	4223.42382(8)	0.3770052(1)	0.14605(5)		87/107	11112f-01101f	3558.69478(8)	P60/R53	87/107	0.26	
11112e	4223.42386(9)	0.3761576(2)	0.13883(5)		82/108	11112e-01101e	3558.69482(9)	P62/R58	82/108	0.26	
11111e	4366.80261(7)	0.37598627(9)	0.11631(2)		101/119	11111e-01101e	3702.07357(7)	P56/R72	101/119	0.32	
11111f	4366.80263(7)	0.3768394(1)	0.11300(3)		104/114	11111f-01101f	3702.07359(7)	P56/R66	104/114	0.32	
00021e	4655.20261(7)	0.3726496(2)	0.12490(6)		105/106	00021e-00001e	4655.20261(7)	P52/R53	105/106	0.19	
00021e	4655.2040(2)	0.372651(43)	0.1250(2)			00021e-00001e	4655.2040(20)				Ref. [22]
20013e	4821.51464(6)	0.3763888(2)	0.1694(1)	0.37(3)	170/188	20013e-10002e 20013e-00001e	3549.22817(6) 4821.51464(6)	P38/R51 P59/R61	53/67 117/121	0.46 0.16	
20013e	4821.5154(7)	0.376396(3)	0.1716(15)			20013e-00001e	4821.5154(73)				Ref. [22]
20012e	4939.36166(5)	0.3750838(2)	0.1216(1)	0.72(2)	219/252	20012e-10001e 20012e-10002e 20012e-00001e	3563.33433(5) 3667.07519(5) 4939.36166(5)	P33/R37 P53/R48 P59/R62	33/52 67/78 119/122	0.55 0.4 0.25	
20012e	4939.3606(31)	0.375119(16)	0.163(18)			20012e-00001e	4939.3606(31)				Ref. [22]
12211e	5035.5207(1)	0.3770957(3)	0.1337(1)		48/58	12211e-02201e	3705.6726(1)	P34/R49	48/58	0.42	Perturbed
12211f	5035.5207(1)	0.3770906(3)	0.1170(1)		46/64	12211f-02201f	3705.6726(1)	P33/R50	46/64	0.42	Perturbed
20011e	5068.92467(5)	0.3762639(2)	0.0915(2)	0.40(3)	250/270	20011e-10001e 20011e-10002e 20011e-00001e	3692.89734(5) 3796.63820(5) 5068.92467(5)	P35/R52 P43/R45 P57/R58	55/68 81/86 114/116	0.39 0.3 0.15	
20011e	5068.9268(5)	0.3762637(13)	0.0905(6)			20011e-00001e	5068.9268(5)				Ref. [22]
01121f	5295.0795(1)	0.3736762(4)	0.1279(3)		37/41	01121f-00001e	5295.0795(1)	Q41	37/41	0.38	
01121e	5295.0800(1)	0.3731230(6)	0.1244(5)		45/49	01121e-00001e	5295.0800(1)	P24/R35	45/49	0.38	
21113e	5439.3001(1)	0.3764414(7)	0.1495(9)	1.3(3)	71/82	21113e-01101e	4774.5711(1)	P43/R42	71/82	0.34	
21113f	5439.30020(9)	0.3776053(3)	0.1644(2)		75/83	21113f-01101f	4774.57116(9)	P44/R42	75/83	0.34	
21112e	5593.66803(9)	0.3755652(2)	0.1230(1)		62/89	21112e-01101e 21112e-01101e	4928.93899(9) 4928.9672	P52/R42	62/89	0.38	Perturbed
21112f	5593.66824(9)	0.3766094(2)	0.12437(9)		60/85	21112f-01101f 21112f-01101f	4928.93920(9) 4929.0698	P54/R41	60/85	0.38	Perturbed
21111f	5756.53626(9)	0.3773184(3)	0.1014(2)		73/81	21111f-01101f	5091.80722(9)	P42/R43	73/81	0.25	
21111e	5756.53639(9)	0.3761187(2)	0.1064(1)		75/84	21111e-01101e	5091.80735(9)	P41/R46	75/84	0.25	
30014e	6033.47610(9)	0.3770392(4)	0.1914(3)		68/68	30014e-00001e	6033.47610(9)	P35/R37	68/68	0.36	
30014e	6033.4786(3)	0.3770422(16)	0.1933(14)			30014e-00001e	6033.4786(3)				Ref. [22]
30014e	6033.47696(33)	0.37703945(90)	0.19187(44)		56/65	30014e-00001e	6033.47696(33)	P50/R48	56/65		Ref. [23]
30013e	6175.95133(7)	0.3749829(3)	0.1539(4)	1.1(1)	148/156	30013e-10002e 30013e-00001e	4903.66486(7) 6175.95133(7)	P39/R42 P49/R49	51/58 97/98	0.4 0.21	
30013e	6175.95270	0.37497775(49)	0.14929(15)		83/90	30013e-00001e	6175.95270(30)	P47/R61	83/90		Ref. [23]
30013e	6175.9545(2)	0.374982(65)	0.1512(4)			30013e-00001e	6175.9545(2)				Ref. [22]

30012e	6298.11219(8)	0.3753131(4)	0.0899(4)	0.5(1)	129/142	30012e-10001e 30012e-00001e	4922.08486(8) 6298.11219(8)	P35/R34 P46/R50	33/45 96/97	0.39 0.21	
30012e	6298.11455	0.37531111(60)	0.08865(24)		86/87	30012e-00001e	6298.11455(28)	P54/R54	86/87		Ref. [23]
30012e	6298.1155(1)	0.375313(52)	0.0888(4)			30012e-00001e	6298.1155(1)				Ref. [22]
30011e	6463.48061(9)	0.3767523(3)	0.0671(2)		75/75	30011e-00001e	6463.48061(9)	P39/R40	75/75	0.42	
30011e	6463.48141	0.3767514(11)	0.06691(59)		72/81	30011e-00001e	6463.48141(34)	P45/R45	72/81		Ref. [23]
30011e	6463.4838(4)	0.376758(4)	0.0798(10)			30011e-00001e	6463.4838(4)				Ref. [22]
31113f	6810.8937(2)	0.376656(1)	0.136(1)		27/41	31113f-01101f	6146.1647(2)	P30/R30	27/41	0.46	
31113f	6811.27330	0.3766456(27)	0.1304(19)		24/26	31113f-01101f	6146.16752(60)	P15/R38	24/26		Ref. [23]
31113f	6810.89654(66)	0.3766464(27)	0.1307(19)		30/32	31113f-01101f	6146.16740(66)	P36/R39	30/32		Ref. [24]
31113e	6810.8945(2)	0.375347(1)	0.123(1)		33/47	31113e-01101e	6146.1655(2)	P30/R30	33/47	0.46	
31113e	6811.27141	0.3753431(21)	0.1235(14)		29/30	31113e-01101e	6146.16694(50)	P17/R37	29/30		Ref. [23]
00031e	6945.59725(7)	0.3696709(1)	0.12450(5)		107/110	00031e-00001e	6945.59725(7)	P54/R57	107/110	0.27	
00031e	6945.6017(4)	0.369673(2)	0.1256(17)			00031e-00001e	6945.6017(4)				Ref. [22]
31112e	6972.7276(2)	0.375466(1)	0.112(1)		26/39	31112e-01101e	6307.9986(2)	P29/R31	26/39	0.55	
31112e	6973.10717	0.3754542(23)	0.1048(21)		41/44	31112e-01101e	6308.00258(48)	P33/R34	41/44		Ref. [23]
31112f	6972.7296(2)	0.376794(1)	0.102(1)		23/39	31112f-01101f	6308.0006(2)	P29/R31	23/39	0.55	
31112f	6973.10817	0.3767914(27)	0.1023(20)		33/36	31112f-01101f	6308.00224(51)	P39/R17	33/36		Ref. [23]
01131f	7573.0911(2)	0.370710(2)	0.117(4)	-7(3)	43/56	01131f-01101f	6908.3621(2)	P33/R33	43/56	1.21	
01131e	7573.0928(2)	0.370182(2)	0.141(3)	5(2)	43/59	01131e-01101e	6908.3638(2)	P33/R33	43/59	1.21	
10032e	8154.4647(4)	0.370044(2)	0.145(1)		56/68	10032e-00001e	8154.4647(4)	P38/R38	56/68	1.39	
10031e	8254.3915(4)	0.369679(2)	0.105(1)		57/68	10031e-00001e	8254.3915(4)	P39/R34	57/68	1.36	

<sup>a</sup>  $N_{tot}$  is the total number of observed transitions reaching a given vibrational state and  $n_{tot}$  is the number of them included in the fit.

<sup>b</sup>  $\Delta G_v = G'_v - G''_v$ .

<sup>c</sup> Observed branch with the maximum value of the total angular momentum quantum number.

<sup>d</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.

<sup>e</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{ cm}^{-1}$ .

<sup>f</sup> The references are given for the bands studied by other authors.

<sup>g</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.

**Table 5**  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed bands of  $^{17}\text{O}^{12}\text{C}^{17}\text{O}$  in this work.

State ( $V_1 V_2 I_2 V_3 r \varepsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	$n_{\text{tot}}/N_{\text{tot}}^a$	Fitted bands	$\Delta G_v^b$	Observed lines <sup>c</sup>	$n/N^d$	RMS <sup>e</sup>	Notes <sup>f</sup>
11102e	1900.25400(9) <sup>g</sup>	0.3675262(2)	0.1311(2)	0.08(3)	98/98	11102e-00001e	1900.25400(9)	P63/R63	98/98	0.22	
11102f	1900.2541(1)	0.3683146(3)	0.1362(1)		44/45	11102f-00001e	1900.2541(1)	Q47	44/45	0.22	
11101e	2048.12284(7)	0.3676466(2)	0.1114(1)	0.07(2)	98/102	11101e-00001e	2048.12284(7)	P69/R49	98/102	0.17	
11101f	2048.1229(1)	0.3685252(2)	0.10766(8)		48/53	11101f-00001e	2048.1229(1)	Q54	48/53	0.17	
00011e	2330.59282(6)	0.36430342(5)	0.117765(9)		134/153	00011e-00001e	2330.59282(6)	P81/R84	134/153	0.28	
00011e	2330.592955(9)	0.36430339(10)	0.117781(27)	0.039(20)	74	00011e-00001e	2330.592955(9)	P66/R69	74		Ref. [15]
12201e	2726.7263(1)	0.3686850(4)	0.1304(3)	-0.65(6)	66/72	12201e-01101e	2064.6598(1)	P59/R12	53/56	0.34	
						12201e-01101f	2064.6598(1)	Q43	13/16	0.34	
12201f	2726.72633(8)	0.3686850(2)	0.11286(7)		65/70	12201f-01101f	2064.65983(8)	P56/R12	50/54	0.34	
						12201f-01101e	2064.65983(8)	Q35	15/16	0.34	
20001e	2755.4992(1)	0.3680611(3)	0.0848(1)		36/38	20001e-01101e	2093.4327(1)	P49	36/38	0.29	
01111f	2980.28699(8)	0.36528279(9)	0.12028(2)		90/129	01111f-01101f	2318.22049(8)	P71/R69	90/129	0.39	
01111f	2980.284794(67)	0.36528122(22)	0.11901(18)	-0.32(4)		01111f-01101f		P59/R51	44		Ref. [15]
01111e	2980.28747(8)	0.3647475(1)	0.11938(2)		93/132	01111e-01101e	2318.22097(8)	P70/R69	93/132	0.39	
01111e	2980.284794(67)	0.36474687(22)	0.11866(18)	-0.21(4)		01111e-01101e		P59/R58	42		Ref. [15]
21103e	3124.7704(1)	0.3676330(2)	0.14288(8)		59/79	21103e-00001e	3124.7704(1)	P50/R53	59/79	0.37	
21102e	3278.4862(1)	0.3671636(2)	0.11791(4)		90/96	21102e-00001e	3278.4862(1)	P61/R55	90/96	0.29	
21102f	3278.4864(2)	0.3681900(9)	0.1159(7)		25/31	21102f-00001e	3278.4864(2)	Q36	25/31	0.29	
						10012e-10001e	2203.53146(5)	P39	20/32	0.52	
10012e	3568.47183(5)	0.3643151(1)	0.13633(8)	0.14(1)	205/249	10012e-10002e	2310.23639(5)	P53/R54	56/86	0.48	
						10012e-00001e	3568.47183(5)	P71/R65	129/131	0.28	
02211f	3630.40365(9)	0.3657223(2)	0.12206(6)		59/93	02211f-02201f	2305.86746(9)	P59/R43	59/93	0.36	
02211e	3630.40373(8)	0.3657220(2)	0.12491(5)		65/93	02211e-02201e	2305.86755(8)	P59/R43	65/93	0.36	
						10011e-10001e	2307.75702(4)	P59/R55	57/93	0.4	
10011e	3672.69739(4)	0.3646005(1)	0.10066(6)	0.080(8)	245/304	10011e-10002e	2414.46195(4)	P34/R44	61/79	0.45	
						10011e-00001e	3672.69739(4)	P65/R73	127/132	0.28	
11112e	4198.18517(7)	0.3647280(1)	0.13030(5)		89/105	11112e-01101e	3536.11867(7)	P64/R46	89/105	0.35	
11112f	4198.18520(7)	0.3655044(1)	0.13654(4)		91/108	11112f-01101f	3536.11870(7)	P65/R47	91/108	0.35	
11111e	4343.44602(8)	0.3647819(2)	0.10971(8)		78/91	11111e-01101e	3681.37952(8)	P51/R51	78/91	0.32	
11111f	4343.44627(9)	0.3656142(2)	0.10659(8)		75/90	11111f-01101f	3681.37977(9)	P52/R49	75/90	0.32	
20013e	4787.57223(7)	0.3647603(2)	0.1581(2)	0.30(3)	113/122	20013e-00001e	4787.57223(7)	P61/R60	113/122	0.14	
12212e	4833.2904(2)	0.365903(3)	0.18(1)	172(13)	28/33	12212e-02201e	3508.7542(2)	P27/R19	28/33	0.39	
12212f	4833.2905(2)	0.365903(3)	0.18(1)	172(13)	28/33	12212f-02201f	3508.7543(2)	P27/R19	28/33	0.39	
20012e	4901.03337(6)	0.3638724(2)	0.1100(1)	0.97(3)	156/181	20012e-10001e	3536.09300(6)	P44/R40	41/57	0.53	
						20012e-00001e	4901.03337(6)	P62/R63	115/124	0.26	
20011e	5039.36881(6)	0.3651627(2)	0.0866(1)	0.37(3)	159/173	20011e-10002e	3781.13337(6)	P24/R37	48/53	0.43	
						20011e-00001e	5039.36881(6)	P63/R62	111/120	0.23	
21113e	5402.02936(9)	0.3649102(2)	0.1418(1)		67/80	21113e-01101e	4739.96286(9)	P48/R34	67/80	0.34	
21113f	5402.02968(8)	0.3659728(2)	0.1537(1)		67/79	21113f-01101f	4739.96318(8)	P49/R33	67/79	0.34	
21112f	5554.53875(8)	0.3653099(2)	0.1157(1)		71/83	21112f-01101f	4892.47225(8)	P43/R50	71/83	0.32	
21112e	5554.53880(8)	0.3643172(2)	0.11528(7)		64/79	21112e-01101e	4892.47230(8)	P42/R53	64/79	0.32	
21111f	5723.47742(9)	0.3661670(3)	0.0966(2)		65/78	21111f-01101f	5061.41092(9)	P45/R42	65/78	0.3	



2111e	5723.47769(8)	0.3649886(3)	0.1006(2)	66/74	21111e-01101e	5061.41119(8)	P45/R43	66/74	0.3
30014e	5988.91296(9)	0.3653501(3)	0.1777(2)	71/76	30014e-00001e	5988.91296(9)	P43/R39	71/76	0.38
30013e	6122.70458(8)	0.3635284(4)	0.1358(4)	98/101	30013e-00001e	6122.70458(8)	P49/R51	98/101	0.24
30013e	6122.71039(39)	0.36352341(85)	0.13119(30)	96	30013e-00001e	6122.71039(39)	<i>J</i> <sup>max</sup> =54	96	Ref. [25]
30012e	6249.95059(8)	0.3643224(3)	0.0833(1)	79/80	30012e-00001e	6249.95059(8)	P43/R43	79/80	0.24
30011e	6425.2063(2)	0.3656644(7)	0.0620(5)	62/69	30011e-00001e	6425.2063(2)	P40/R40	62/69	0.8
31113e	6757.4389(3)	0.364007(1)	0.1162(8)	43/52	31113e-01101e	6095.3724(3)	P38/R34	43/52	1.05
31113f	6757.4398(3)	0.365213(1)	0.123(1)	39/42	31113f-01101f	6095.3733(3)	P32/R32	39/42	1.05
00031e	6917.81966(7)	0.3585279(1)	0.11727(5)	88/93	00031e-00001e	6917.81966(7)	P57/R38	88/93	0.27
01131f	7542.8508(2)	0.3595353(8)	0.1183(9)	33/54	01131f-01101f	6880.7843(2)	P33/R31	33/54	1.04
01131e	7542.8562(2)	0.3590205(8)	0.1186(8)	34/54	01131e-01101e	6880.7897(2)	P33/R31	34/54	1.04
10032e	8114.654784(7)	0.35873938(3)	0.14761(2)	75/75	10032e-00001e	8114.654784(7)	P37/R37	75/75	0.03
10031e	8215.040718(7)	0.35872244(4)	0.09851(4)	65/65	10031e-00001e	8215.040718(7)	P35/R29	65/65	0.03

<sup>a</sup>  $N_{tot}$  is the total number of observed transitions reaching a given vibrational state and  $n_{tot}$  is the number of them included in the fit.

<sup>b</sup>  $\Delta G_v = G_v - G_v^*$ .

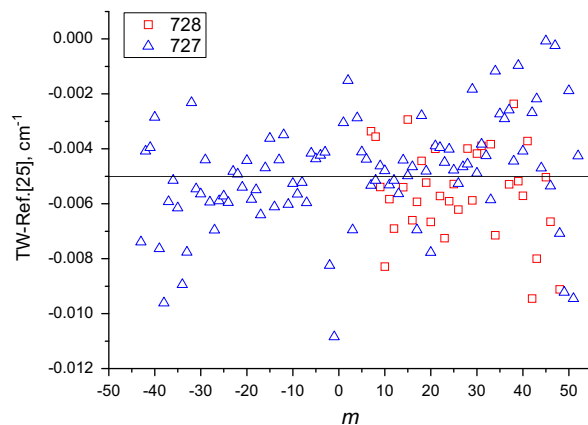
<sup>c</sup> Observed branch with the maximum value of the total angular momentum quantum number.

<sup>d</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.

<sup>e</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{ cm}^{-1}$ .

<sup>f</sup> The references are given for the bands studied by other authors.

<sup>g</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.



**Fig. 4.** Differences between our measured line positions (TW) and those published in Ref. [25] versus  $m$  (where  $m = -J$  for P-branch and  $m = J + 1$  for R-branch). Open squares stand for the transitions of the 30013-00001 band of  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$ . Open triangles stand for the transitions of the 30013-00001 band of  $^{17}\text{O}^{12}\text{C}^{17}\text{O}$ .

references and spectroscopic constants of other authors (in italics) for the bands earlier observed. For the fitting of the spectroscopic constants of the upper states the spectroscopic constants for the lower states taken from Ref. [15] have been used. Note that two of the observed bands, namely 12211-02201 and 21112-01101, are perturbed. The lines of these bands near the energy level crossings were removed from the fits. The analysis of the perturbation mechanisms will be given in Section 6. It should be emphasised that among the earlier observed bands 7 of them were observed only in the Venus spectra [22].

### $^{17}\text{O}^{12}\text{C}^{17}\text{O}$

From 35 assigned bands for this isotopologue only 3 bands were observed before [15,25]. The spectroscopic constants for all these observed bands are given in Table 5. They were obtained in the results of the fits with the use of the lower states spectroscopic constants from Ref. [15]. The band 01131-01101 is found to be perturbed. The lines of this band near the energy level crossing were removed from the fit. For the comparison the spectroscopic constants from other authors for three earlier observed bands are also presented in italics in Table 5. There is rather good agreement between our measured line positions and those published in Ref. [15] for the 00011-00001 and 01111-01101 bands. But our measured line positions for 30013-00001 band are shifted by about  $0.005 \text{ cm}^{-1}$  from those of Ref. [25]. The respective comparison is presented in Fig. 4 for this band.

### $^{17}\text{O}^{12}\text{C}^{18}\text{O}$

29 bands of this isotopologue in LADIR and USTC spectra were assigned, 18 of which were observed for the first time. In Table 6 we present spectroscopic constants for all observed bands. These constants were obtained in the results of the fits of the line positions using the spectroscopic constants for the lower states

**Table 6**  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed bands of  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  in this work.

State ( $V_1 V_2 I_2 V_3 r \varepsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	$n_{\text{tot}}/N_{\text{tot}}^a$	Fitted bands	$\Delta G_v^b$	Observed lines <sup>c</sup>	$n/N^d$	RMS <sup>e</sup>	Notes <sup>f</sup>
11102f	1884.7237(1) <sup>g</sup>	0.3579109(3)	0.1277(1)		43/44	11102f-00001e	1884.7237(1)	Q47	43/44	0.15	
11102e	1884.72374(9)	0.3571851(2)	0.12285(6)		53/53	11102e-00001e	1884.72374(9)	P57	53/53	0.15	
11101f	2036.0384(1)	0.3583429(2)	0.1025(1)		44/48	11101f-00001e	2036.0384(1)	Q51	44/48	0.19	
11101e	2036.03840(6)	0.3574870(1)	0.10526(4)		75/78	11101e-00001e	2036.03840(6)	P60/R26	75/78	0.19	
00011e	2322.43440(5)	0.35412378(5)	0.111291(8)		143/158	00011e-00001e	2322.43440(5)	P85/R82	143/158	0.23	
00011e	2322.434478(10)	0.354123815(92)	0.111292(18)		82	00011e-00001e	2322.434478(10)	P71/R69	82		Ref. [15]
00011e	2322.434472(13)	0.35412360(10)	0.111262(26)		33	00011e-10001e		P33/R32	33		Ref. [18]
00011e	2322.434472(13)	0.35412360(10)	0.111262(26)		53	00011e-10002e		P45/R45	53		Ref. [18]
00011e	2322.43504(15)	0.35412305(12)	0.111161(23)		65	00011e-00001e	2322.43504(15)	J'max=74	65		Ref. [26]
20003e	2473.49064(6)	0.3569528(2)	0.14545(7)		96/97	20003e-00001e	2473.49064(6)	P50/R48	96/97	0.27	
20002e	2585.66725(7)	0.3566519(2)	0.09918(7)		93/95	20002e-00001e	2585.66725(7)	P51/R43	93/95	0.26	
20001e	2738.24115(7)	0.3579641(3)	0.0811(2)		73/73	20001e-00001e	2738.24115(7)	P40/R35	73/73	0.34	
01111f	2969.82660(7)	0.3550717(1)	0.11355(3)		86/117	01111f-01101f	2310.12494(7)	P68/R57	86/117	0.39	
01111f	2969.823927(48)	0.35507173(16)	0.11349(12)	-0.02(2)		01111f-01101f					Ref. [15]
01111e	2969.82685(7)	0.3545640(1)	0.11285(2)		86/117	01111e-01101e	2310.12519(7)	P68/R57	86/117	0.39	
01111e	2969.823927(48)	0.35456415(16)	0.11292(12)	0.02(2)		01111e-01101e					Ref. [15]
21103e	3097.2727(2)	0.3572128(4)	0.1345(2)		26/38	21103e-00001e	3097.2727(2)	R47	26/38	0.47	
21102e	3251.1295(1)	0.3569841(2)	0.11044(7)		68/82	21102e-00001e	3251.1295(1)	P51/R54	68/82	0.39	
10012e	3547.28098(5)	0.3540018(1)	0.12712(6)	0.147(8)	176/215	10012e-10002e	2302.68685(5)	P54/R48	45/73	0.46	
10012e	3547.28119(11)	0.35400088(11)	0.12467(33)		89	10012e-00001e	3547.28098(5)	P76/R71	131/142	0.22	
10012e						10012e-00001e	3547.28119(11)	J'max=62	89		Ref. [26]
02211f	3617.65298(8)	0.3555077(2)	0.1153(1)		53/71	02211f-02201f	2297.83422(8)	P49/R47	53/71	0.42	
02211e	3617.65304(8)	0.3555075(2)	0.1196(1)		52/71	02211e-02201e	2297.83428(8)	P49/R47	52/71	0.42	
10011e	3655.12232(5)	0.35456535(8)	0.09568(2)		156/183	10011e-10001e	2299.46810(5)	P52/R47	41/60	0.42	
10011e	3655.12232(5)	0.35456535(8)	0.09568(2)			10011e-00001e	3655.12232(5)	P66/R63	115/123	0.23	
10011e	3655.12238(7)	0.35456536(10)	0.095817(35)		68	10011e-00001e	3655.12238(7)	J'max=59	68		Ref. [26]
30003e	3811.33155(9)	0.3560572(3)	0.1155(2)		64/67	30003e-00001e	3811.33155(9)	P37/R39	64/67	0.41	
11112e	4175.06865(7)	0.3544619(1)	0.12267(3)		92/111	11112e-01101e	3515.36699(7)	P64/R56	92/111	0.37	
11112e	4175.07700(24)	0.35446214(38)	0.122956(165)		53	11112e-01101e	3515.3672	J'max=50	53		Ref. [26]
11112f	4175.06896(7)	0.3551769(1)	0.12786(3)		91/111	11112f-01101f	3515.36730(7)	P64/R58	91/111	0.37	
11112f	4175.07698(24)	0.35517770(25)	0.128127(115)		64	11112f-01101f	3515.3672	J'max=48	64		Ref. [26]
11111e	4323.23665(9)	0.3547055(3)	0.1043(2)		57/72	11111e-01101e	3663.53499(9)	P45/R40	57/72	0.31	
11111e	4323.24477(19)	0.35470600(36)	0.10475(15)		40	11111e-01101e	3663.5355	J'max=48	40		Ref. [26]
11111f	4323.23679(9)	0.3555181(3)	0.1016(2)		61/72	11111f-01101f	3663.53513(9)	P43/R39	61/72	0.31	
11111f	4323.24520(24)	0.35551623(31)	0.10004(12)		41	11111f-01101f	3663.5355	J'max=55	41		Ref. [26]
00021e	4620.32961(7)	0.3513181(2)	0.11115(8)		91/93	00021e-00001e	4620.32961(7)	P49/R45	91/93	0.28	
20013e	4755.55871(7)	0.3543032(2)	0.1478(2)		116/122	20013e-00001e	4755.55871(7)	P61/R59	116/122	0.21	
20013e	4755.55905(6)	0.35430287(9)	0.147165(37)		83	20013e-00001e	4755.55905(6)	J'max=51	83		Ref. [26]
12212e	4808.0365(2)	0.355591(2)	0.153(6)	79(5)	42/48	12212e-02201e	3488.2177(2)	P30/R29	42/48	0.42	
12212f	4808.0367(2)	0.355589(2)	0.141(6)	73(5)	40/48	12212f-02201f	3488.2179(2)	P30/R29	40/48	0.42	
20012e	4866.90142(7)	0.3538303(2)	0.1007(2)	1.13(4)	111/117	20012e-00001e	4866.90142(7)	P58/R61	111/117	0.18	
20012e	4866.90158(5)	0.35383008(12)	0.100417(113)		83	20012e-00001e	4866.90158(5)	J'max=55	83		Ref. [26]
20011e	5013.94548(6)	0.3551543(2)	0.08101(9)		92/93	20011e-00001e	5013.94548(6)	P47/R46	92/93	0.21	
20011e	5013.94552(15)	0.35515495(30)	0.0811498(196)		50	20011e-00001e	5013.94552(15)	J'max=42	50		Ref. [26]
21113f	5367.42353(9)	0.3555256(4)	0.1447(3)		58/69	21113f-01101f	4707.72187(9)	P38/R32	58/69	0.3	

21113e	5367.42399(9)	0.3545553(4)	0.1336(3)	60/70	21113e-01101e	4707.72233(9)	P38/R33	60/70	0.3
21112f	5519.49935(9)	0.3551666(3)	0.1083(1)	59/76	21112f-01101f	4859.79769(9)	P50/R41	59/76	0.3
21112f	5519.50620(75)	0.35517296(272)	0.11439(294)	33	21112f-01101f	4859.7973	$J_{\max}=30$	33	Ref. [26]
21112e	5519.49957(8)	0.3542160(2)	0.1080(1)	62/81	21112e-01101e	4859.79791(8)	P49/R43	62/81	0.3
21112e	5519.50775(75)	0.35421768(292)	0.10934(300)	27	21112e-01101e	4859.7973	$J_{\max}=31$	27	Ref. [26]
21111f	5694.7810(1)	0.3561218(5)	0.0915(4)	40/55	21111f-01101f	5035.0793(1)	P38/R29	40/55	0.4
21111e	5694.7810(1)	0.3549686(5)	0.0955(4)	42/54	21111e-01101e	5035.0793(1)	P37/R30	42/54	0.4
30014e	5946.97862(9)	0.3548205(3)	0.1666(2)	68/73	30014e-00001e	5946.97862(9)	P40/R40	68/73	0.43
30013e	6073.76098(8)	0.3533126(2)	0.1172(1)	70/93	30013e-00001e	6073.76098(8)	P50/R50	70/93	0.41
30013e	6073.7669(12)	0.3533107(29)	0.1160(12)	40	30013e-00001e	6073.7669(12)		40	Perturbed Ref. [25]
30012e	6207.7606(1)	0.3544101(4)	0.0783(3)	61/64	30012e-00001e	6207.7606(1)	P37/R36	61/64	0.4
00031e	6893.71258(6)	0.3485146(1)	0.11080(4)	91/106	00031e-00001e	6893.71258(6)	P59/R56	91/106	0.29

<sup>a</sup>  $N_{\text{tot}}$  is the total number of observed transitions reaching a given vibrational state and  $n_{\text{cor}}$  is the number of them included in the fit.

<sup>b</sup>  $\Delta G_v = G_v - G_v'$ .

<sup>c</sup> Observed branch with the maximum value of the total angular momentum quantum number.

<sup>d</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.

<sup>e</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{ cm}^{-1}$ .

<sup>f</sup> The references are given for the bands studied by other authors.

<sup>g</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.

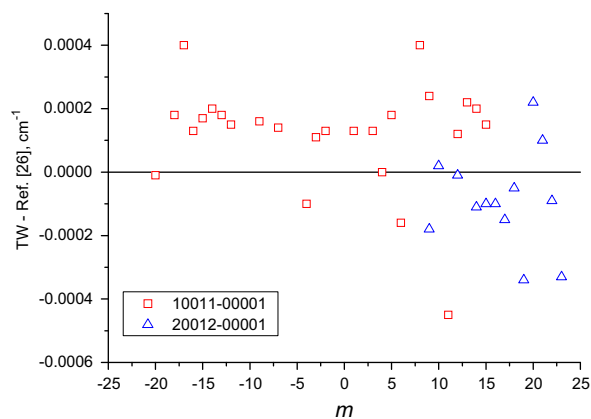


Fig. 5. Differences between our measured line positions (TW) and those published in Ref. [26] versus  $m$  (where  $m = -J$  for P-branch and  $m = J + 1$  for R-branch) for 10011-00001 and 20011-00001 bands of  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$ .

taken from Ref. [15]. The majority of the known bands of  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  were observed in Ref. [26]. Our line positions are in a good agreement with those published in Ref. [26]. This is demonstrated in Fig. 5 where for the comparison two bands 10011-00001 and 20012-00001 are chosen. But the term values  $G_v$  for the upper states 11111, 11112 and 21112 recovered in Ref. [26] from the line positions of the hot bands 11111-01101, 11112-01101 and 21112-01101 differ slightly from ours ( $\text{TW} - \text{Ref. [26]} = -0.008 \text{ cm}^{-1}$ ) whereas the  $\Delta G_v$  values are in a good agreement. It is due to the fact that in Ref. [26] the constants for lower state 01101 are not determined. Again our line positions for 30013-00001 band are shifted by about  $0.005 \text{ cm}^{-1}$  from those of Ref. [25] (see Fig. 4). The upper vibrational state of this band is found to be perturbed by the interpolyad anharmonic resonance interaction with vibrational state 50006. The energy level crossing is at  $J = 33$ .

### $^{16}\text{O}^{13}\text{C}^{17}\text{O}$

8 bands of this isotopologue in the studied spectra were assigned, 3 of which were observed for the first time. The spectroscopic constants for all observed bands are presented in Table 7. They were fitted to the observed line positions with the use of the lower states constants from Ref. [27]. The fundamental band 00011-00001 was studied in Ref. [27]. Two bands, namely the 10011-00001 and 10012-00001 bands, were observed in Ref. [14] and two bands 20011-00001 and 20012-00001 were studied in Ref. [28]. Our line positions for these bands agree with those from Refs. [14,27,28] within  $0.001 \text{ cm}^{-1}$ .

### $^{17}\text{O}^{13}\text{C}^{17}\text{O}$

Among 7 assigned bands for this isotopologue only one band 00011-00001 was observed before [27]. Our observed line positions for this band agree within  $0.0005 \text{ cm}^{-1}$  with those published in Ref. [27]. The spectroscopic constants for all these observed bands are presented in Table 8. These constants were obtained from the results of the fits of the line

**Table 7**  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed bands of  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  in this work.

State ( $V_1 V_2 I_2 V_3 r \varepsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	Fitted bands	$\Delta G_v^a$	Observed lines <sup>b</sup>	$n/N^c$	RMS <sup>d</sup>	Notes <sup>e</sup>
11101 f	2020.1919(2) <sup>f</sup>	0.3794272(8)	0.1153(7)		11101f-00001e	2020.1919(2)	Q35	25/27	0.26	
11101e	2020.1922(1)	0.3785775(2)	0.11861(7)		11101e-00001e	2020.1922(1)	P57	51/52	0.26	
00011e	2274.08705(7)	0.3757535(2)	0.12577(7)	0.229(9)	00011e-00001e	2274.08705(7)	P78/R58	111/136	0.34	
00011e	2274.08706(1)	0.37575373(43)	0.12594(35)	0.27(7)	00011e-00001e	2274.08706(1)	P55/R50	62		Ref.[27]
01111f	2908.17789(8)	0.3767358(1)	0.12653(3)		01111f-01101f	2262.43128(8)	P67/R43	72/102	0.4	
01111e	2908.17791(9)	0.3761550(1)	0.12591(4)		01111e-01101e	2262.43130(9)	P66/R43	64/98	0.4	
10012e	3508.37386(7)	0.3763522(2)	0.14732(6)		10012e-00001e	3508.37386(7)	P55/R47	90/98	0.36	
10012e	3508.37379(50)	0.376349(2)	0.1449(15)		10012e-00001e	3508.37379(50)	$J^{\text{max}}=37$	26		Ref.[14]
10011e	3608.54972(7)	0.3753797(2)	0.10973(7)		10011e-00001e	3608.54972(7)	P47/R53	80/89	0.31	
10011e	3608.54946(18)	0.3753820(6)	0.11106(11)		10011e-00001e	3608.54946(18)	$J^{\text{max}}=48$	34		Ref.[14]
11112f	4124.3975(1)	0.3774359(4)	0.1464(3)		11112f-01101f	3478.6509(1)	P41/R31	44/53	0.39	
11112e	4124.3981(1)	0.3764938(4)	0.1367(3)		11112e-01101e	3478.6515(1)	P41/R31	46/57	0.39	
20012e	4849.39217(8)	0.3752435(2)	0.1369(1)		20012e-00001e	4849.39217(8)	P45/R49	70/80	0.33	
20012e	4849.39270(12)	0.37523329(25)	0.134907(95)		20012e-00001e	4849.39270(12)	P54/R54	94/97		Ref.[28]
20011e	4955.59010(9)	0.3755578(3)	0.0904(1)		20011e-00001e	4955.59010(9)	P38/R45	57/68	0.39	
20011e	4955.59042(11)	0.37554895(27)	0.08915(12)		20011e-00001e	4955.59042(11)	P47/R59	81/84		Ref.[28]

<sup>a</sup>  $\Delta G_v = G'_v - G''_v$ .

<sup>b</sup> Observed branch with the maximum value of the total angular momentum quantum number.

<sup>c</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.

<sup>d</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{cm}^{-1}$ .

<sup>e</sup> The references are given for the bands studied by other authors.

<sup>f</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.

**Table 8**  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed in this work bands of  $^{17}\text{O}^{13}\text{C}^{17}\text{O}$ .

State ( $V_1 V_2 I_2 V_3 r \varepsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	Fitted bands	$\Delta G_v^a$	Observed lines <sup>b</sup>	$n/N^c$	RMS <sup>d</sup>	Notes <sup>e</sup>
11101e	2004.1402(1) <sup>f</sup>	0.3673008(3)	0.1113(1)		11101e-00001e	2004.1402(1)	P51	43/43	0.3	
11101f	2004.1409(1)	0.3681311(5)	0.1075(4)		11101f-00001e	2004.1409(1)	Q38	32/37	0.3	
00011e	2264.35930(6)	0.36442837(5)	0.117757(9)		00011e-00001e	2264.35930(6)	P85/R62	130/140	0.31	
00011e	2264.35948(2)	0.36442822(41)	0.11765(21)	-0.03(2)	00011e-00001e	2264.35948(2)	P55/R46	68		Ref. [27]
01111e	2895.77312(8)	0.3648298(1)	0.12079(3)		01111e-01101e	2252.77100(8)	P72/R48	79/115	0.41	
01111f	2895.77327(8)	0.3653788(1)	0.12036(2)		01111f-01101f	2252.77115(8)	P72/R48	87/116	0.41	
10012e	3487.80234(7)	0.3648570(1)	0.13836(3)		10012e-00001e	3487.80234(7)	P69/R49	94/113	0.38	
10011e	3584.89594(8)	0.3642394(2)	0.10142(9)		10011e-00001e	3584.89594(8)	P49/R49	75/82	0.38	
11112e	4100.56184(9)	0.3650604(2)	0.13257(9)		11112e-01101e	3457.55972(9)	P54/R31	62/75	0.36	
11112f	4100.56184(9)	0.3659272(2)	0.13812(8)		11112f-01101f	3457.55972(9)	P53/R31	68/78	0.36	
20012e	4810.69381(9)	0.3638803(2)	0.1233(1)		20012e-00001e	4810.69381(9)	P48/R47	65/82	0.32	
00031e	6723.7153(2)	0.3588688(8)	0.1213(7)		00031e-00001e	6723.7153(2)	35/35	71/71	0.74	

<sup>a</sup>  $\Delta G_v = G'_v - G''_v$ .

<sup>b</sup> Observed branch with the maximum value of the total angular momentum quantum number.

<sup>c</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.

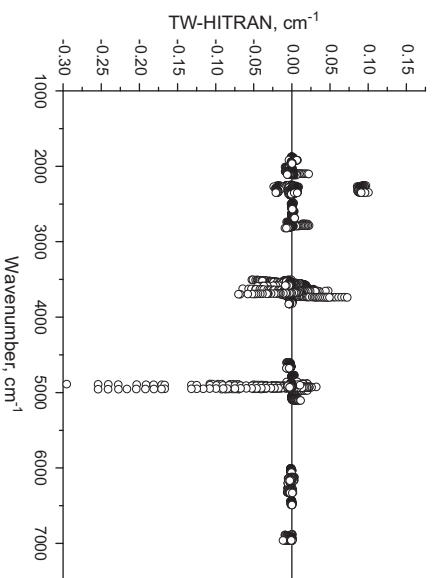
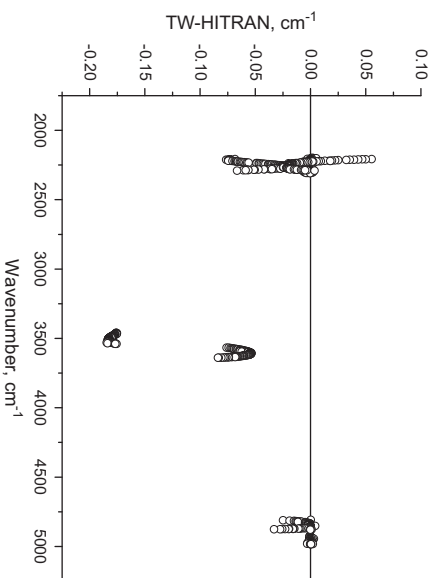
<sup>d</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{cm}^{-1}$ .

<sup>e</sup> The references are given for the bands studied by other authors.

<sup>f</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.

**Table 9**Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the observed in this work bands of  $^{17}\text{O}^{13}\text{C}^{18}\text{O}$ .

State ( $V_1V_2 I_2 V_3 r \varepsilon$ )	$G_v$	$B_v$	$D_v \times 10^6$	$H_v \times 10^{12}$	Fitted bands	$\Delta G_v^a$	Observed lines <sup>b</sup>	$n/N^c$	RMS <sup>d</sup>	Notes <sup>e</sup>
00011e	2255.95371(7) <sup>f</sup>	0.3542408(2)	0.11083(7)	-0.198(8)	00011e-00001e	2255.95371(7)	P80/R65	118/139	0.31	
00011e	2255.95383(2)	0.35424080(84)	0.11088(71)	-0.18(16)	00011e-00001e	2255.95383(2)	P49/R50	62		Ref.[27]
01111f	2884.99102(9)	0.3551636(1)	0.11495(3)		01111f-01101f	2244.42718(9)	P66/R47	73/106	0.44	
01111e	2884.99111(8)	0.3546409(1)	0.11326(3)		01111e-01101e	2244.42727(8)	P66/R47	79/102	0.44	
10012e	3468.65285(7)	0.3545103(1)	0.13090(3)		10012e-00001e	3468.65285(7)	P67/R47	105/114	0.31	
10011e	3564.6164(1)	0.3542253(3)	0.0950(2)		10011e-00001e	3564.6164(1)	P46/R42	47/63	0.39	
11112f	4078.73742(9)	0.3555753(2)	0.1310(1)		11112f-01101f	3438.17358(9)	P51/R28	68/74	0.36	
11112e	4078.73753(9)	0.3547742(2)	0.1241(1)		11112e-01101e	3438.17369(9)	P51/R27	61/71	0.36	
20012e	4775.4826(1)	0.3537086(5)	0.1114(3)		20012e-00001e	4775.4826(1)	P38/R38	46/58	0.38	

<sup>a</sup>  $\Delta G_v = G_v - G_v'$ .<sup>b</sup> Observed branch with the maximum value of the total angular momentum quantum number.<sup>c</sup>  $N$  is the number of the observed lines for a given branch(es) and  $n$  is the number of these lines included in the fit.<sup>d</sup> Root Mean Squares of residuals of the spectroscopic parameters fit is given in  $10^{-3} \text{cm}^{-1}$ .<sup>e</sup> The references are given for the bands studied by other authors.<sup>f</sup> Between parentheses, the confidence interval (1 SD) is in the units of the last quoted digit.**Fig. 6.** Differences between our measured line positions (TW) and those contained in HITRAN2008 for  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  isotopologue of carbon dioxide.**Fig. 7.** Differences between our measured line positions (TW) and those contained in HITRAN2008 for  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologue of carbon dioxide.**Table 10**  
Observed interpolyad perturbations.

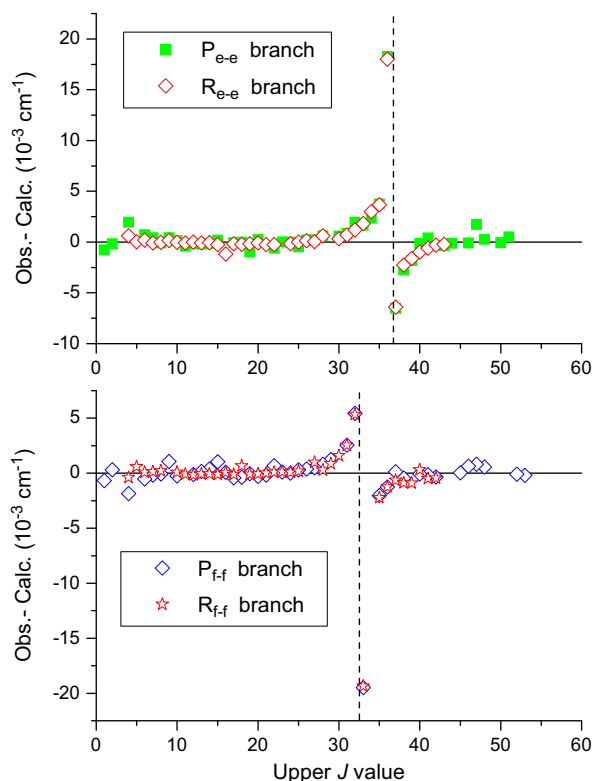
Isotopologue	Band affected	Center ( $\text{cm}^{-1}$ )	Perturber <sup>a</sup>	$J_{\text{pert}}^b$
$^{16}\text{O}^{12}\text{C}^{17}\text{O}$	12211-02201	3705.67	32204	e: 90, f: 97
$^{16}\text{O}^{12}\text{C}^{17}\text{O}$	21112-01101	4928.94	41105	e: 37, f: 33
$^{17}\text{O}^{12}\text{C}^{18}\text{O}$	30013-00001	6073.76	50006	33

<sup>a</sup> HITRAN labeling for the vibrational states.<sup>b</sup> Value of the angular momentum quantum number at which the energy level crossing takes place.

positions using the spectroscopic constants for the lower state taken from Ref. [27].

 $^{17}\text{O}^{13}\text{C}^{18}\text{O}$ 

Again among 6 assigned bands for this isotopologue only one band 00011-00001 was observed before [27]. Our observed line positions for this band also agree within  $0.0005 \text{cm}^{-1}$  with those published in Ref. [27]. The spectroscopic constants for all observed bands are presented in



**Fig. 8.** Residuals between observed and calculated line positions for the 21112-01101 band of  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ . Upper panel: e-e subband. Lower panel: f-f subband.

**Table 9.** They were fitted to the observed line positions with the use of the lower state constants from Ref. [27].

## 5. Comparison with HITRAN database

The HITRAN2008 database [4] contains the calculated line parameters for many bands of the rare isotopologues of carbon dioxide. Because of this it is very interesting to compare our observed line positions to those from HITRAN2008. In Fig. 6 such comparison for  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  isotopologue is presented. One can see from this figure that for several bands there exist very large differences between observed and HITRAN line positions. First of all we have to mention the 21112-01101 band centered at  $4928.94\text{ cm}^{-1}$  which originates from OCO database [29]. The differences reach  $-0.3\text{ cm}^{-1}$ . The HITRAN line positions for the 02211-02201 band centered at  $2315.15\text{ cm}^{-1}$  deviate from the measured ones by about  $0.09\text{ cm}^{-1}$ . This band originates from the old version of the CDSD-296 databank [30].

In Fig. 7 the comparison of our observed line positions to those contained in HITRAN2008 is presented for  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologue. The HITRAN line positions for the 10011-00001 band centered at  $3608.54\text{ cm}^{-1}$  and for the 10012-00001 band centered at  $3508.37\text{ cm}^{-1}$  deviate from the observed ones by about  $0.06\text{ cm}^{-1}$  and  $0.18\text{ cm}^{-1}$  respectively. These bands originate from CDSD-296 calculated values [1]. The

calculations were performed with the effective Hamiltonian parameters of Ref. [8] which were slightly refined in Ref. [6].

## 6. Discussion and conclusion

In this paper the extensive information about line positions of the carbon dioxide isotopologues in the  $1700\text{--}8300\text{ cm}^{-1}$  wavenumber region was obtained. In total 239 bands of 12 isotopologues were observed and analyzed. Among them 99 bands were observed for the first time. The positions of 23,003 lines were determined with the experimental uncertainty on the level of  $0.001\text{ cm}^{-1}$ . The spectroscopic constants were fitted to the observed line positions for all observed bands. The mean value of the RMS of all fittings is about  $0.0003\text{ cm}^{-1}$ . It was shown that several bands of  $^{17}\text{OCO}$  isotopologues have to be updated in HITRAN database. The measured line positions of this work will be used for the improvement of the  $\text{CO}_2$  spectra modeling within the framework of the method of effective operators. It is planned to perform new fittings of the effective Hamiltonian parameters for  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$ ,  $^{17}\text{O}^{12}\text{C}^{17}\text{O}$ ,  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  and  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  isotopologues. Then the obtained sets of the effective Hamiltonian parameters will be used for the refinement of the CDSD databank.

In addition to the cases published in Refs. [6,31–33], three new cases of the interpolyad anharmonic resonance interactions have been observed in  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  and  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  asymmetric isotopologues. They are gathered in Table 10. The respective perturbations for the 21112–01101 band of  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  are illustrated in Fig. 8 where the residuals between observed and calculated line positions are plotted versus the total angular momentum quantum number  $J$ . In spite of the fact that there exist the interpolyad resonance perturbations in the case of asymmetric isotopologues the polyad model of effective Hamiltonian for the  $\text{CO}_2$  molecule works very well. The interpolyad resonance interactions seldom take place and for the symmetric isotopologues they were never observed.

## Acknowledgments

This work is jointly supported by RFBR (Russia, Grants Nos. 10-05-93105 and 10-05-91176), CNRS (France) and CAS (China) in the frame of Groupement de Recherche International SAMIA (Spectroscopie d’Absorption des Molécules d’Intérêt Atmosphérique). OML acknowledges the support by RFBR (Grant RFBR 09-05-92508-ИК\_а) and CRDF (Grant RUG1-2954-TO-09).

## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.jqsrt.2012.06.028>.

## References

- [1] Perevalov VI, Tashkun SA. CDSD-296 (Carbon Dioxide Spectroscopic Databank): updated and enlarged version for atmospheric applications.

- In: Proceedings of the 10th HITRAN database conference, Cambridge, MA, USA, <ftp://ftp.iaa.ru/pub/CDS-2008/>; 2008.
- [2] Tashkun SA, Perevalov VI, Teffo JL, Bykov AD, Lavrentieva NN. CDS-1000, the high-temperature carbon dioxide spectroscopic databank. *J Quant Spectrosc Radiat Transfer* 2003;82:165–96.
  - [3] Tashkun SA, Perevalov VI. CDS-4000: high-resolution, high-temperature carbon dioxide spectroscopic databank. *J Quant Spectrosc Radiat Transfer* 2011;112:1403–10.
  - [4] Rothman LS, Gordon LE, Barbe A, Chris Benner D, Bernath PF, Birk M, et al. The HITRAN 2008 molecular spectroscopic database. *J Quant Spectrosc Radiat Transfer* 2009;110:533–72.
  - [5] Tashkun SA, Perevalov VI, Teffo JL. Global fittings of the vibrational-rotational line positions of the  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  and  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  isotopic species of carbon dioxide. *J Mol Spectrosc* 2001;210:137–45.
  - [6] Perevalov BV, Kassi S, Romanini D, Perevalov VI, Tashkun SA, Campargue A. Global effective Hamiltonians of  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$  and  $^{16}\text{O}^{13}\text{C}^{18}\text{O}$  improved from CW-CRDS observations in the 5900–7000  $\text{cm}^{-1}$  region. *J Mol Spectrosc* 2007;241:90–100.
  - [7] Jacquemart D, Gueye F, Lyulin OM, Karlovets EV, Baron D, Perevalov VI. Infrared spectroscopy of  $\text{CO}_2$  isotopologues from 2200 to 7000  $\text{cm}^{-1}$ : I—characterizing experimental uncertainties of positions and intensities. *J Quant Spectrosc Radiat Transfer* 2012;113:961–75.
  - [8] Chedin A. The carbon dioxide molecule. Potential, spectroscopic, and molecular constants from its infrared spectrum. *J Mol Spectrosc* 1979;76:430–91.
  - [9] Chedin A, Teffo JL. The carbon dioxide molecule: a new derivation of the potential, spectroscopic, and molecular constants. *J Mol Spectrosc* 1984;107:333–42.
  - [10] Rothman LS, Hawkins RL, Wattson RB, Gamache RR. Energy levels, intensities, and linewidths of atmospheric carbon dioxide bands. *J Quant Spectrosc Radiat Transfer* 1992;48:537–66.
  - [11] Wilquet V, Mahieux A, Vandaele AC, Perevalov VI, Tashkun SA, Fedorova A, et al. Line parameters for the 01111–00001 band of  $^{12}\text{C}^{16}\text{O}^{18}\text{O}$  from SOIR measurements of the Venus atmosphere. *J Quant Spectrosc Radiat Transfer* 2008;109:895–905.
  - [12] Villanueva G, Mumma MJ, Novak R, Hewagama T. Discovery of multiple bands of isotopic  $\text{CO}_2$  in the prime spectral regions used when searching for  $\text{CH}_4$  and  $\text{H}_2\text{O}$  on Mars. *J Quant Spectrosc Radiat Transfer* 2008;109:883–94.
  - [13] Robert S, Borkov Yu, Vander Auwera J, Drummond R, Mahieux A, Wilquet V, et al. Assignment and rotational analysis of new absorption bands of carbon dioxide isotopologues in Venus spectra. *J Quant Spectrosc Radiat Transfer*, submitted. <http://dx.doi.org/10.1016/j.jqsrt.2012.08.023>, in press.
  - [14] Toth RA, Miller CE, Brown LR, Malathy Devi V, Benner DC. 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  $\text{cm}^{-1}$ . *J Mol Spectrosc* 2008;251:64–89.
  - [15] Claveau C, Teffo JL, Hurtmans D, Valentin A. Infrared fundamental and first hot bands of  $\text{O}^{12}\text{C}^{17}\text{O}$  isotopic variants of carbon dioxide. *J Mol Spectrosc* 1998;189:153–95.
  - [16] Rinsland CP, Benner DC, Malathy Devi V. Measurements of absolute line intensities in carbon dioxide bands near 5.2  $\mu\text{m}$ . *Appl Opt* 1985;24:1644–50.
  - [17] Rinsland CP, Benner DC. Absolute intensities of spectral lines in carbon dioxide bands near 2050  $\text{cm}^{-1}$ . *Appl Opt* 1984;23:4523–8.
  - [18] Claveau C, Teffo JL, Hurtmans D, Valentin A, Gamache RR. Line positions and absolute intensities in the laser bands of carbon-12 oxygen-17 isotopic species of carbon dioxide. *J Mol Spectrosc* 1999;193:15–32.
  - [19] Guelachvili G. High-resolution Fourier spectra of carbon dioxide and three of its isotopic species near 4.3  $\mu\text{m}$ . *J Mol Spectrosc* 1980;79:72–83.
  - [20] Malathy Devi V, Rinsland CP, Benner DC. Absolute intensity measurements of  $\text{CO}_2$  bands in the 2395–2680  $\text{cm}^{-1}$  region. *Appl Opt* 1984;23:4067–75.
  - [21] Rinsland CP, Benner DC, Malathy Devi V. Absolute line intensities in  $\text{CO}_2$  bands near 4.8  $\mu\text{m}$ . *Appl Opt* 1986;25:1205–14.
  - [22] Mandin JY. Interpretation of the  $\text{CO}_2$  absorption bands observed in the Venus infrared spectrum between 1 and 2.5  $\mu\text{m}$ . *J Mol Spectrosc* 1977;67:304–21.
  - [23] Majcherova Z, Macko P, Romanini D, Perevalov VI, Tashkun SA, Teffo JL, et al. High-sensitivity CW-cavity ringdown spectroscopy of  $^{12}\text{CO}_2$  near 1.5  $\mu\text{m}$ . *J Mol Spectrosc* 2005;230:1–21.
  - [24] Perevalov BV, Kassi S, Romanini D, Perevalov VI, Tashkun SA, Campargue A. CW-cavity ringdown spectroscopy of carbon dioxide isotopologues near 1.5  $\mu\text{m}$ . *J Mol Spectrosc* 2006;238:231–55.
  - [25] de Ghellinck d'Elseghem Vaernewijck X, Kassi S, Herman M.  $^{17}\text{O}^{12}\text{C}^{17}\text{O}$  and  $^{18}\text{O}^{12}\text{C}^{17}\text{O}$  overtone spectroscopy in the 1.64  $\mu\text{m}$  region. *Chem Phys Lett* 2011;514:29–31.
  - [26] Toth RA, Miller CE, Brown LR, Malathy Devi V, Benner DC. Line positions and strengths of  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ ,  $^{18}\text{O}^{12}\text{C}^{18}\text{O}$  and  $^{17}\text{O}^{12}\text{C}^{18}\text{O}$  between 2200 and 7000  $\text{cm}^{-1}$ . *J Mol Spectrosc* 2007;243:43–61.
  - [27] Teffo JL, Claveau C, Valentin A. Infrared fundamental bands of  $\text{O}^{13}\text{C}^{17}\text{O}$  isotopic variants of carbon dioxide. *J Quant Spectrosc Radiat Transfer* 1998;59:151–64.
  - [28] Ding Y, Macko P, Romanini D, Perevalov VI, Tashkun SA, Teffo JL, et al. High sensitivity cw-cavity ringdown and Fourier transform absorption spectroscopies of  $^{13}\text{CO}_2$ . *J Mol Spectrosc* 2004;226:146–60.
  - [29] Toth RA, Brown LR, Miller CE, Malathy Devi V, Benner DC. Spectroscopic database of  $\text{CO}_2$  line parameters: 4300–7000  $\text{cm}^{-1}$ . *J Quant Spectrosc Radiat Transfer* 2008;109:906–21.
  - [30] Tashkun SA, Perevalov VI, Teffo JL, Bykov AD, Lavrentieva NN. CDS-296 the carbon dioxide spectroscopic databank: version for atmospheric application. In: Proceedings of the XIVth symposium on high resolution molecular spectroscopy, Krasnoyarsk, Russia; 2003.
  - [31] Perevalov BV, Kassi S, Perevalov VI, Tashkun SA, Campargue A. High sensitivity CW-cavity ring down spectroscopy of  $^{12}\text{C}^{16}\text{O}_2$ ,  $^{16}\text{O}^{12}\text{C}^{17}\text{O}$  and  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  between 5851 and 7045  $\text{cm}^{-1}$ : line position analysis and critical review of the current databases. *J Mol Spectrosc* 2008;252:143–59.
  - [32] Perevalov BV, Perevalov VI, Campargue A. A (nearly) complete experimental linelist for  $^{13}\text{C}^{16}\text{O}_2$ ,  $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ ,  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ ,  $^{13}\text{C}^{18}\text{O}_2$  and  $^{17}\text{O}^{13}\text{C}^{18}\text{O}$  by high-sensitivity CW-CRDS spectroscopy between 5851 and 7045  $\text{cm}^{-1}$ . *J Quant Spectrosc Radiat Transfer* 2008;109:2437–62.
  - [33] Campargue A, Song KF, Mouton N, Perevalov VI, Kassi S. High sensitivity CW-cavity ring down spectroscopy of five  $^{13}\text{CO}_2$  isotopologues of carbon dioxide in the 1.26–1.44  $\mu\text{m}$  region (I): line positions. *J Quant Spectrosc Radiat Transfer* 2010;111:659–74.