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Atlas of new and revised high-resolution spectroscopy of six CO isotopologues in the 101–115 nm range

Transition energies of the $v' = 0, 1, 2,$ and 3 to $v'' = 0$ bands of the $B^1\Sigma^+, C^1\Sigma^+,$ and $E^1\Pi$ to $X^1\Sigma^+$ states, related term values, and molecular constants

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ABSTRACT

Our knowledge of astronomical environments containing CO depends on accurate molecular data to reproduce and interpret observed spectra. The recent and future improvements of ultraviolet space instrumentation, both in sensitivity and resolution, require increasingly detailed laboratory molecular spectroscopy as a reference. As part of a long-term experimental campaign at the SOLEIL Synchrotron facility, we have acquired gas-phase absorption spectra of six CO isotopologues in the vacuum ultraviolet. These spectra are recorded using the Fourier-transform spectrometer installed on the DESIRS beamline, providing a unique resolving power up to 10^6 in the 8–13 eV range. We have used resolutions in the 300 000–450 000 range for this campaign, which enable the analysis of individual line positions. We report new measurements on neighboring Rydberg states in the 101–115 nm range that could also be used as f -value calibrators, namely $B^1\Sigma^+, C^1\Sigma^+,$ and $E^1\Pi$, for six CO isotopologues. This range encompasses the absorption transitions $B(v' = 0, 1, \text{ and } 2), C(v' = 0, 1, 2, \text{ and } 3),$ and $E(v' = 0, 1, 2, \text{ and } 3)$ from $X^1\Sigma^+(v'' = 0)$. Higher resolution laser-based measurements of CO isotopologues from the literature are used to improve the absolute calibration and accuracy of our data. The overall uncertainty of the great majority of the line positions presented in this atlas is estimated to be 0.01 cm^{-1} . In addition, some of the data derived from transition energies measurements, such as term values and molecular constants, are obtained for the first time, and others are improvements on previous sparser or lower spectral resolution datasets.

Key words. molecular data – methods: laboratory: molecular – techniques: spectroscopic – techniques: interferometric

1. Introduction

This work is part of a larger effort to catalog, interpret, and model the photoabsorption spectrum of CO in the 90–155 nm wavelength region. These measurements are performed at the third-generation SOLEIL synchrotron facility in Saint-Aubin, France. We employ the Fourier-transform spectrometer (FTS) installed on the DESIRS beam line, a unique instrument that combines high spectral resolution and a high signal-to-noise ratio (S/N) in the vacuum ultraviolet (VUV) wavelength range.

In the course of our earlier work (2008–2015) on CO photoabsorption spectroscopy in the 90–155 nm region, we were mainly interested in oscillator strengths and perturbations for several CO isotopologues. A large part of this work concerned the Rydberg W – X bands and Rydberg complexes in the 92.5–97.5 nm range: Eidelsberg et al. (2012, 2014, 2017) for $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, and $^{13}\text{C}^{18}\text{O}$, respectively, and perturbations

in the W – X bands (Heays et al. 2014) and the f -value measurements of the lowest VUV states (Stark et al. 2014), while another part dealt with the A – X bands for $^{13}\text{C}^{16}\text{O}$ (Gavilan et al. 2013) and $^{13}\text{C}^{18}\text{O}$ (Lemaire et al. 2016). The common goal of these studies was the accurate determination of oscillator strengths, with an absolute calibration made by reference to the unperturbed $B^1\Sigma^+(v' = 0)$ – $X^1\Sigma^+(v'' = 0)$ band that was previously well characterized by high-resolution (0.14 cm^{-1}) laser-based measurements (Stark et al. 1999) and by synchrotron-based measurements (Federman et al. 2001). The $B^1\Sigma^+$ – $X^1\Sigma^+$ bands were already extensively investigated for four isotopologues ($^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, and $^{13}\text{C}^{18}\text{O}$) in both absorption and emission (Eidelsberg et al. 1987) using the Observatoire de Paris (Meudon, France) 10 m VUV grating spectrograph. In that work, term values were derived for the B00, B10, and B20 absorption bands. The uncertainty on the absolute wavenumbers was estimated to be $\pm 0.1 \text{ cm}^{-1}$.

Throughout this paper, the notation is simplified as follows: states are designed by their symmetry (e.g., $X^1\Sigma^+$ or $E^1\Pi$), while a band is denoted $E^1\Pi(v')$ – $X^1\Sigma^+(v'')$ or for brevity $EXv'v''$, for

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example, EX20 for $v' = 2$ and $v'' = 0$, or shorter: E20. The notation indicating the isotopologues is also simplified in tables and figures, where we write, for example, 1216 for $^{12}\text{C}^{16}\text{O}$, etc.

The current investigation describes our high-resolution measurements of the $B^1\Sigma^+$, $C^1\Sigma^+$, and $E^1\Pi$ states for six CO isotopologues in the 101–115 nm range. This range encompasses the following absorption transitions: $B(v' = 0, 1 \text{ and } 2)$, $C(v' = 0, 1, 2 \text{ and } 3)$, and $E(v' = 0, 1, 2 \text{ and } 3)$ from the fundamental electronic state $X(v'' = 0)$.

This work revisits and completes, 25 yr later, part of the CO atlas of transition frequencies started by the Paris-Meudon Observatory team (Eidelsberg et al. 1991; Le Floch 1992), and initiated by the work of Letzelter et al. (1987) and Viala et al. (1988) on the photoabsorption and photodissociation cross sections, either measured or calculated for the four isotopologues $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$. It improves and completes calculations derived from the combination of earlier low-resolution measurements of term values and molecular constants of B00 and B10 for $^{12}\text{C}^{16}\text{O}$ (Le Floch & Amiot 1985), of C00 and E00 for $^{12}\text{C}^{16}\text{O}$ (Le Floch 1992), and of B00, B10, C00 and E00 for $^{12}\text{C}^{18}\text{O}$ and $^{13}\text{C}^{18}\text{O}$ (Haridass et al. 1994). Line positions of B20 for $^{12}\text{C}^{16}\text{O}$ have been studied by Baker & Launay (1994).

This work also revisits and completes earlier experimental work at low resolution on E00 and E10 (Baker et al. 1993, 1994). Higher resolution work (Cacciani et al. 1995, 2001; Cacciani & Ubachs 2004; Drabbels et al. 1993a,b; Ubachs et al. 1995, 2000) is discussed in detail in Sect. 2.1 as these data are used in this work for the absolute calibration of our data.

It is also worth mentioning the extensive work of Morton & Noreau (1994), which provides a compilation of electronic transitions (including BX00 to BX20, CX00 to CX30, and EX00 to EX20) in the CO molecule ($^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$). Line positions are limited in this work to $J'' \leq 6$. This paper includes all experimental data published up to 1994.

A first detailed model of CO photodissociation, based on laboratory data, including depth-dependent attenuation and isotope-selective self-shielding of photodissociation rates, was developed by van Dishoeck & Black (1988) to model in detail, coupled with a chemical network, the structure and chemistry of a variety of interstellar clouds. This work, updated by measurements produced in the subsequent 20 yr, was revisited by Visser et al. (2009), including self- and mutual-shielding of all isotopologues (in particular, for the first time, $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$) as well as shielding by atomic and molecular hydrogen.

All term values are referenced to the $X^1\Sigma^+(v'' = 0, J'' = 0)$ ground state of the respective isotopologues, according to the ground-state energy levels determined by Guelachvili et al. (1983) and Farrenq et al. (1991).

This work only reports and is based on lines that are observed and clearly identified in spectra, with the exception of the extremely congested Q -branches of the E state (at low J) for which we report in our tables literature values obtained at very high resolution (for E00 and E10) or estimated (for E20) for the sake of completeness.

This article is organized as follows. Section 2 briefly describes the experimental setup and the analysis procedure. Section 3 presents our results: line assignments, term values, and molecular constants for each state (B , C , and E) and bands observed. The last section presents our concluding remarks.

2. Experimental setup and data analysis

CO spectra are recorded at high resolution using the vacuum-ultraviolet Fourier-transform spectrometer (VUV-FTS) available on beamline DESIRS (Dichroïsme Et Spectroscopie par Interaction avec le Rayonnement Synchrotron) of the SOLEIL synchrotron. The beamline and spectrometer have been described in detail in previous publications (de Oliveira et al. 2009, 2011, 2016; Nahon et al. 2012, 2013).

Four bottles of isotopically purified gases, namely $^{12}\text{C}^{16}\text{O}$ (Alphagaz, 99.997%), $^{12}\text{C}^{18}\text{O}$ (ICON Isotopes, ^{18}O 99%), $^{13}\text{C}^{16}\text{O}$ (Messer, ^{13}C 99.1%; ^{16}O 99.95%), $^{13}\text{C}^{18}\text{O}$ (Cambridge Isotopes, ^{13}C 99%, ^{18}O 95%), and one bottle containing a $^{12}\text{C}^{16}\text{O}/^{12}\text{C}^{17}\text{O}/^{12}\text{C}^{18}\text{O}$ mixture (ICON Isotopes, 41.5%, 48.5%, and 9.9% respectively), are used to obtain data for five isotopologues. The presence of a sixth isotopologue, the rarely studied $^{13}\text{C}^{17}\text{O}$, is detected as an impurity in the $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$ bottles, and serves to complete this analysis, which provides a consistent dataset on six natural isotopologues.

Sample gases continuously flow through a 10 cm long windowless absorption cell that is open on both sides through capillary tubes. Most spectra are recorded at room temperature (295 K), but a few are obtained with the central part of the cell cooled by liquid nitrogen; this results in a gas temperature of 90 ± 5 K. In some cases, these cooled spectra are useful for improved line assignments by reducing the number of lines in a spectrum and their Doppler broadening.

A total of 69 spectra, recorded at different pressures and spectral resolutions, were analyzed for this work (amounting to 3327 individual lines). The analysis was performed line by line, determining the line positions by modeling them as Gaussian or Voigt functions (for $\sim 97\%$ of the cases), and at times extracting them from simulations of the spectra of blended lines. In order to improve the accuracy, the present results rely on up to four different records for a given band and a given isotopologue. The bands observed in this work are reported in Table 1.

A key element of this work is the need for absolute wavelength calibration. The first step in the calibration procedure is provided by the FTS team. In summary, the raw FTS interferogram data based on the accurate measurement of the mirror displacement are first phase-corrected and then Fourier-transformed into a frequency spectrum. The resulting spectra are frequency-calibrated using atomic lines from different origins that appear in the spectra (de Oliveira et al. 2011, 2016). The accuracy of individual rovibrational lines is not only dependent on the accuracy of the absolute frequency calibration atomic lines, but also on the spectral resolution and on the strength and blendedness of each measured line. The parameters involved are the number, N , of independent scanning steps for a given line, which depends itself on the width, W , (mainly Doppler) of the measured line, and on the S/N compared to the background continuum signal. The final accuracy of line positions, σ in wavenumbers, reported by de Oliveira et al. (2011), is based on the empirical expression $\Delta(\sigma) \sim W/(S/N \times \sqrt{N})$ (see also their reference 20).

Lemaire et al. (2016) reported line positions determined from VUV-FTS spectra with a relative accuracy better than $\sim \pm 0.008 \text{ cm}^{-1}$ at $87\,000 \text{ cm}^{-1}$ (or $\sim \pm 0.01 \text{ pm}$ at 115 nm). A comparison of wavenumber measurements of common sets of lines from multiple independent spectra is consistent with this estimated accuracy.

Two methods were used to place all spectra on a unique wavelength scale. First, more than 30 atomic lines (mainly Xe I, Kr I, and sometimes O I) present in the studied range were

Table 1. Summary of bands measured at high resolution.

Isotopologue	State	$B^1\Sigma^+$			$C^1\Sigma^+$			$E^1\Pi$					
	Band	BX			CX			EX					
	$v'-v''$	$v=0$	00	10	20	00	10	20	30	00	10	20	30
$^{12}\text{C}^{16}\text{O}$	*	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
$^{12}\text{C}^{17}\text{O}$	*	✓	✓	no	✓	✓	no	✓	✓	✓	✓	✓	✓
$^{12}\text{C}^{18}\text{O}$	*	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
$^{13}\text{C}^{16}\text{O}$	*	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
$^{13}\text{C}^{17}\text{O}$	*	✓	✓	no	✓	✓	no	no	✓	✓	no	no	no
$^{13}\text{C}^{18}\text{O}$	*	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

Notes. ✓: observed, no: not observed. * are data calculated from Farrenq et al. (1991).

Table 2. References to the high-resolution calibration band or lines used (reference labels sorted by publication dates are given at the bottom of the table).

Isotopologue	State	$B^1\Sigma^+$			$C^1\Sigma^+$			$E^1\Pi$				
	Band	BX			CX			EX				
	$v'v''$	00	10	20	00	10	20	30	00	10	20	30
$^{12}\text{C}^{16}\text{O}$	$b_{l\bullet}, c_{l\bullet}, j_l$	$c_{l\bullet}$	$a_{b\bullet}$	$b_{l\bullet}, e_{\bullet}, j_l$	$e_{\bullet}, g_{b\bullet}$			$d_{l\bullet}, h_{b\bullet}, j_l$	$a_{\bullet}, d_{l\bullet}, f_b$			
$^{12}\text{C}^{17}\text{O}$				$e_{l\bullet}$	g_l			d_{\bullet}	f_b			
$^{12}\text{C}^{18}\text{O}$	$c_{l\bullet}$			e_{\bullet}	$e_{\bullet}, g_{b\bullet}$			a_{\bullet}, d_{\bullet}	$a_{\bullet}, d_{\bullet}, f_b$			
$^{13}\text{C}^{16}\text{O}$	$c_{l\bullet}, k_{\bullet}$			e_{\bullet}	$e_{\bullet}, g_{b\bullet}$			$a_{\bullet}, d_{\bullet}, h_{b\bullet}$	$a_{\bullet}, d_{\bullet}, f_b$			
$^{13}\text{C}^{17}\text{O}$					g_l				f_b			
$^{13}\text{C}^{18}\text{O}$					$g_{b\bullet}$			$a_{\bullet}, h_{l\bullet}$	a_{\bullet}, f_b			

Notes. References providing data for bands with fewer than about ten lines are indexed with l and for more than ten lines with b . References providing term values and/or molecular constants are indexed with a filled blue dot.

References. a: Baker et al. (1993, 1994); Baker (1994). b: Drabbels et al. (1993a). c: Drabbels et al. (1993b). d: Cacciani et al. (1995). e: Ubachs et al. (1995). f: Ubachs et al. (2000). g: Cacciani et al. (2001). h: Cacciani & Ubachs (2004). j: Daprà et al. (2016). k: Niu et al. (2016).

used with reference frequencies taken from the NIST atomic lines database¹. The presence of these gases is due to unintentional minor contamination or to a column of rare gas introduced on the beamline intended to filter out high-frequency harmonics generated in the undulator. Most of these lines have been measured with an accuracy of 10^{-3} nm and some with an accuracy of up to 10^{-6} nm. These latter are O I: 115.21512 nm (Kaufman & Edlén 1974), Xe I: 106.125564 nm, 105.612829 nm, 104.383497 nm (Yoshino & Freeman 1985; Brandi et al. 2001), and Kr I: 100.1060639 nm (Brandi et al. 2002). The positions of these lines are shown in Fig. 1.

Second, the random error associated with calibrating the wavenumber scale via a small number of atomic transitions can sometimes be improved upon by including reference data for molecular lines. For this aim, high-resolution laser measurements of some CO lines (and isotopologues) available in the literature were employed (Cacciani et al. 1995, 2001; Cacciani & Ubachs 2004; Drabbels et al. 1993a,b; Ivanov et al. 2008; Philip et al. 2004; Ubachs et al. 1994, 1995, 2000, and recently Daprà et al. 2016). Most of these measurements, obtained by narrow-band laser spectroscopy in one- or two-photon experiments, rely on the I₂- or Te₂-saturation spectrum as primary absolute calibrators, associated with the marks of an actively stabilized Fabry-Pérot étalon. They are summarized in the next subsection (in alphabetical order) and are cited in the corresponding sections.

¹ http://physics.nist.gov/PhysRefData/ASD/lines_form.html

To overcome the lack of calibration data for some bands, we considered the overlapping regions of contiguous scans. A given setting of the undulator delivers a quasi-Gaussian beam profile of width ~ 5 nm at $1/e$ of the peak signal. An absorption scan encompasses about 3–5 bands, as can be seen in Fig. 1. With the right choice of undulator settings, we were able to measure at least three bands in a single scan. In this way, a band with no calibration reference can be surrounded by two bands subject to accurate calibration, for instance, the B20 band surrounded by the B10 and C00 bands.

The final accuracy of our measurements also relied upon isotopologue cross calibrations. These were obtained through mixed isotopologue samples (as is the case for the available $^{12}\text{C}^{16}\text{O}$ – $^{12}\text{C}^{17}\text{O}$ bottle, which contains some small amount of $^{12}\text{C}^{18}\text{O}$, and as in the case of $^{13}\text{C}^{17}\text{O}$, which was present as an impurity in $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$ bottles). Even with pure gas samples, isotopologue impurities may show up in spectra that were recorded at high pressures. We also prepared and used on purpose mixed isotopologue samples allowing for such cross calibrations.

It is worth noting that more data were collected for this work than are included in papers dedicated to oscillator strength measurements. Those are restricted in pressure range and consequently in number of lines observed, in order to keep optical depths < 1.5 , or absorption lower than 78%, for the accurate determination of oscillator strengths. For this study we used higher pressures in order to observe high J' levels and isotopologues present in small amounts. As described above, we also use cooled gases to remove possible ambiguities.

2.1. Laser calibration benchmarks and associated data

An absolute calibration of lines requires the availability of accurately determined standards, either atomic or molecular, as close as possible to the lines under study. There are many reported laser-based measurements of CO VUV transitions with accurate absolute calibrations based on primary standards. Some previous work has been limited to a few lines of each vibrational band, while others offer almost complete bands for use as comparisons for calibration purposes. Data like this exist for most CO isotopologues. They are summarized in detail in this section.

Reports of laser-based measurements that were used to accurately calibrate our spectra often also presented an analysis of the rotational structure of the bands under study, providing associated data such as term values, reduced term values, and molecular constants. These results are also mentioned in detail in this section as they are compared later to our own results.

Depending on the data available, laser calibrated benchmarks could in some cases be derived from transitions other than the one-photon P , R , and Q transitions of this study. When two-photon O , S , or Q transitions were available, the corresponding one-photon transitions for the R - and P -branches were recalculated by way of term values, taking into account that common- J' term values (TVs) of the excited state calculated from various one- and two-photon transition frequencies, that is, $\text{TV}(O_{J'=i \leftarrow J''=i+2})$, $\text{TV}(P_{J'=i \leftarrow J''=i+1})$, $\text{TV}(Q_{J'=i \leftarrow J''=i})$, $\text{TV}(R_{J'=i \leftarrow J''=i-1})$, and $\text{TV}(S_{J'=i \leftarrow J''=i-2})$, have to be equal.

We summarize below all references providing laser calibration benchmarks that were used for this work, as well as the associated data mentioned above. They are sorted by alphabetical order of authors. With the exception of the first laser high-resolution measurements (Baker et al. at Paris-Meudon Observatory and Drabbels et al. at Nijmegen University), the majority of CO molecular calibration lines used here were measured using ultra-high resolution lasers at VU University Amsterdam (Cacciani et al., Daprà et al., Ivanov et al., Niu et al., and Ubachs et al.).

Baker (1994)

This paper reports some perturbations observed in the B20 state of $^{12}\text{C}^{16}\text{O}$ that are due to the interaction with the $^3\Pi(\text{F}1)$ spin-orbit component of the $k^3\Pi(0)-X^1\Sigma^+(0)$ band. Line positions and term values are given for B20 and kX00.

Baker & Launay (1994)

This paper analyzes the $k^3\Pi(v'=2, 3 \text{ and } 5)-X^1\Sigma^+(0)$ bands, the first one perturbing the E00 band, and the last one the E10 band. Line positions and term values are given for kX20, kX30, and kX50.

Baker et al. (1993, 1994)

These papers provide a study of the E00 and E10 bands for four isotopologues, $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, and $^{13}\text{C}^{18}\text{O}$. Spectra were recorded using 2 + 1 resonantly enhanced multiphoton excitation showing the five rotational branches O , P , Q , R , and S at a resolution of $\sim 0.1 \text{ cm}^{-1}$. Spectra were acquired either separately for each isotopologue or with mixtures of several, and were then separated by time of flight mass spectrometry, in order to obtain an accurate relative calibration between isotopologues. Perturbations of E10 were analyzed. Term values (for three isotopologues of E00 and four of E10) and molecular constants (for E10) are also given for the four isotopologues.

Cacciani & Ubachs (2004)

This paper gives Q -branch transition frequencies of E00 [$Q: J'=1-8$] for $^{12}\text{C}^{16}\text{O}$ and [$Q: J'=1-7$] for $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$. Measured and calculated transition frequencies for E00 of $^{12}\text{C}^{16}\text{O}$ [up to $J'=34$ with gaps] and $^{13}\text{C}^{16}\text{O}$ [up to $J'=42$

with gaps], obtained by three different experimental methods, are accessible as supplementary data.

Cacciani et al. (1995)

This paper provides a few term values for $^{12}\text{C}^{16}\text{O}$ (the E00 band [$J'=31, 41, \text{ and } 44$] and E10 band [$J'=5-13$]), focused in both cases around perturbations. Molecular constants are also determined for $^{12}\text{C}^{16}\text{O}$ (E00 and E10), $^{13}\text{C}^{16}\text{O}$ (E00 and E10), $^{12}\text{C}^{18}\text{O}$ (E00 and E10), and $^{12}\text{C}^{17}\text{O}$ (E00). Transition frequencies were tabulated in a later paper (Cacciani & Ubachs 2004).

Cacciani et al. (2001)

This paper provides transition frequencies for R - and P -branch lines of the C10 band for $^{12}\text{C}^{16}\text{O}$ [$R: J'=0-27; P: J'=1-31$], $^{12}\text{C}^{18}\text{O}$ [$R: J'=0-13; P: J'=1-8, 10$], $^{13}\text{C}^{16}\text{O}$ [$R: J'=0-15; P: J'=1-5, 9-20$], $^{13}\text{C}^{18}\text{O}$ [$R: J'=0-5, 8-12; P: J'=1, 3, 5-8$], and a few for $^{12}\text{C}^{17}\text{O}$ [$R: J'=0-2; P: J'=1$] and $^{13}\text{C}^{17}\text{O}$ [$R: J'=0-1, 3-5; P: J'=1-3$]. Molecular constants are also calculated for the six isotopologues, although at lower accuracy for $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$.

Daprà et al. (2016)

This paper is mainly based on data for $^{12}\text{C}^{16}\text{O}$ published by the Amsterdam team over several years and gives measured wavelengths (Tables 6–8; called molecular parameters) for the R and P (and Q for E00) $J'=0-5$ transitions of the B00, C00, and E00 bands. Their results are expressed with an accuracy of up to the sixth digit (in nanometers) and an error bar of between 3 and 13 in units of this digit. The restriction to the lowest rotational states ($J' \leq 5$) is due to the fact that this paper is aimed at the comparison with quasar observations. These data are the most accurate to date. They result from measurements and not from calculations, as can be deduced from the fact that term values for a given level, determined through the R - and P -branches, are not strictly equal.

Drabbels et al. (1993a)

This paper reports observed transition frequencies for $^{12}\text{C}^{16}\text{O}$ of the Q - and S -branch lines of B00 [$J'=0-14$ for Q and $0-1$ for S] and of C00 [$J'=0-6$ for Q and $0-1$ for S]. Corresponding molecular constants are also calculated from these data.

Drabbels et al. (1993b) This paper completes the previous paper with additional measurements of Q lines for B10 [$J'=0-2$], for $^{13}\text{C}^{16}\text{O}$ B00 [$J'=0-2$], and for $^{12}\text{C}^{18}\text{O}$ B00 [$J'=0-1$]. There is also a slight revision of $^{12}\text{C}^{16}\text{O}$ B00 [$J'=0-4$ for Q and $0-1$ for S], but as this paper was submitted earlier than the previous paper, it is not clear which should be considered as the more accurate.

Molecular constants are calculated for these four bands.

Ivanov et al. (2008)

This paper reports “extreme-ultraviolet laser metrology of O I transitions” (about 20 lines in the 94.86–102.82 nm range) that are used for absolute calibration purposes, when oxygen is present, for E20 and higher energy states.

Niu et al. (2016)

While focused on the spectroscopy and perturbation analysis of the $A^1\Pi(v=0)$ state of $^{13}\text{C}^{16}\text{O}$, this paper provides deperturbed molecular constants for B00.

Ubachs et al. (1994)

This paper summarizes the work performed in the 91.2–115 nm range by the Amsterdam and Nijmegen teams over several years, reporting molecular constants for many states of four isotopologues and, of relevance to the present work, for $^{12}\text{C}^{16}\text{O}$ (B00, B10, C00), $^{13}\text{C}^{16}\text{O}$ (B00), and $^{12}\text{C}^{18}\text{O}$ (B00).

Ubachs et al. (1995)

This is a laser spectroscopic study of $^{12}\text{C}^{17}\text{O}$ (observed here for the first time) R - and P -branch lines of C00 [$J'=10-17$ for R and $10-15$ for P] and derived molecular constants. The latter are also

given for C00 and C10 for $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{12}\text{C}^{18}\text{O}$, but no transition frequencies are available.

Ubachs et al. (2000)

This paper reports the transition frequencies of E10 for six isotopologues. For $^{12}\text{C}^{16}\text{O}$ [R : $J' = 0–26$ with three gaps; Q : $J' = 8–21$ with two gaps; P : $J' = 5–28$ with three gaps], $^{12}\text{C}^{18}\text{O}$ [R : $J' = 0–11$; Q : $J' = 8–13$ with one gap; P : $J' = 2–13$ with three gaps], $^{13}\text{C}^{16}\text{O}$ [R : $J' = 0–20$ with five gaps; Q : $J' = 7–23$; P : $J' = 2–20$], $^{13}\text{C}^{18}\text{O}$ [R : $J' = 0–20$ with two gaps; Q : $J' = 1, 18$; no P], a few for $^{12}\text{C}^{17}\text{O}$ [R : $J' = 0–1$; Q : $J' = 1–2$; no P] and for $^{13}\text{C}^{17}\text{O}$ [R : $J' = 0–12$ with six gaps; Q : $J' = 1–12$; P : $J' = 3$]. The very high resolution (up to $\sim 3 \times 10^6$) achieved by a narrow-band laser source allowed assigning the Q -branch lines with an absolute accuracy of 0.003 cm^{-1} for all six natural CO isotopologues. Molecular constants are also derived for the ground-state $X(v'' = 0)$, E10 and the perturbing k60 bands.

References to the available absolute high-resolution calibration band or lines we used are summarized in Table 2 for each band and for each isotopologue. The availability of term values and/or molecular constants derived from the laser-based measurements is also noted in the table.

We also mention the mainly theoretical work of Lefèbvre-Brion & Eidelsberg (2012), which presents molecular constants (T_v and B_v) for E00, E10, E20, and E30 derived from our VUV-FTS high-resolution CO datasets, extracted before the absolute wavelength calibration of this work.

2.2. Data analysis

2.2.1. Atlas of measured wavelengths and wavenumbers

In order to place the atlas on an absolute wavelength scale, we compared our measured data with the entire set of calibration references from Table 2 (including all isotopologues when available). The average of their differences provides the value of a shift that was applied to correct the raw experimental wavelengths. As proof of the accuracy of the data delivered by the VUV-FTS team, this correction was usually very small ($< 3.4 \times 10^{-5} \text{ nm}$ or 0.03 cm^{-1}). Two sets of measured transition energies (including calibration shift corrections from the wavelength standards), R_{ms} and P_{ms} , corresponding to the R - and P -branches (and additionally Q_{ms} for $^1\Pi$ states), were the result from this procedure.

In order to check the quality of our transition energy determinations, we compared for each J' the values of

$$A = R_{(J'=i+1 \leftarrow J'=i)} - P_{(J'=i+1 \leftarrow J'=i+2)} \text{ to those of}$$

$$B = X_{J'=i+2} - X_{J'=i},$$

according to the method of combination differences (Herzberg et al. 1950). For each band and for each J' , we calculated the difference $A-B$ between these two quantities, which we defined as $2 \times \delta_P$.

These differences lead to uncertainties in the term values TV_R and TV_P . Some publications interested in precise term values shared equally for each J' the difference between TV_R and TV_P (or between R and P , in order to calculate corrected transition energies $R_{corr} = (R_{ms} - \delta_P)$ and $P_{corr} = (P_{ms} + \delta_P)$, which produces a single best-term value based on both lines. We did not follow this procedure here, but kept the measured values.

2.2.2. Atlas of term values and molecular constants

For each measured band, we used the line positions of R - and P -branch lines that terminate on the same upper rotational levels to calculate common upper-level term values with uncertainties.

The agreement of the term values calculated from independently measured P - and R -branch transitions with a common upper J -level, TV_R , and TV_P , is never perfect because of experimental noise and in some cases line broadening. However, as we described above, the excellent reproducibility of the measurements obtained with the VUV-FTS for a given band and a given isotopologue from spectra recorded at different times suggests that when the discrepancy is larger than the random fitting errors, it reveals the possible presence of a local perturbation that modifies the shape of one of the lines involved. For each $J' = i + 1$ level, the final term value was obtained by averaging the term values $\text{TV}_R = R_{J'=i+1 \leftarrow J'=i} + X_{J'=i}$ and $\text{TV}_P = P_{J'=i+1 \leftarrow J'=i+2} + X_{J'=i+2}$ that were calculated from measured line positions of each rotational branch, R_{ms} and P_{ms} . The relative difference is again $2 \times \delta_P$. As a final result, R_{ms} , P_{ms} and δ_P values are tabulated for each band and isotopologue. Both R_{ms} and P_{ms} are given in wavelengths and wavenumbers (and δ_P in wavenumbers), and are presented in separate tables for ^{12}C - and ^{13}C -bearing CO species.

Term values of the upper levels for all six isotopologues were derived from these two independent measurements. They are presented in separate tables for each band, while reduced term values are shown with graphs for better visualization. We must be careful for high J' term values in two specific cases: (a) a high value of δ_P (we adopted in this work a limit of 0.125 cm^{-1}) might mean that one of the lines is less well identified than the other (or does not belong to the studied band), even if the two R and P lines are both clearly observed, and (b) no δ_P value indicates that only one transition is present, either R or P . In the first case, we kept the TV derived from a single level, while in the second case, erratic TV values had to be rejected. All these tables and graphs are introduced for each state in the following sections.

For each band and isotopologue, the statistical uncertainty on term values was obtained by calculating over all J' , when both R and P levels were measured, the average and standard deviation (at 2σ) of $2 \times \delta_P/2$. The division by a factor of two takes into account that each term value results from two independent measurements (R_{ms} and P_{ms}) and that at least two different records (up to four in some cases, as described above) provide the same line position results. Each average is displayed in statistical tables, alongside its standard deviation (at 2σ), showing the dispersion in our measurements. An average closer to zero means that the δ_P values are randomly distributed, ensuring no bias in our measurements. A standard deviation closer to zero signifies a high probability of the absence of perturbation(s).

The molecular constants T_v , B_v , and D_v were least-squares fitted to the experimental term values using a second-order polynomial. Following the above remarks, only a subset of term values was considered at times, particularly for high J' term values. Reduced term values were finally calculated for each vibrational level by subtracting a model defined by

$$\text{TV}(J) = T_v + B_v \times J(J+1) - D_v \times J^2(J+1)^2$$

for the e -parity levels of the $B^1\Sigma^+$ and $C^1\Sigma^+$ states and the f -parity levels of the $E^1\Pi$ state, while for the e -parity levels of $E^1\Pi$, the additional term

$$q \times J(J+1) - q_D \times J^2(J+1)^2$$

takes the Λ -doubling of this state into account (so that $q = B_e - B_f$ and $q_D = D_e - D_f$, where the e and f subscripts refer to the parity of the considered levels). For the $E^1\Pi$ state, the Λ -doubling

components can be either calculated by subtracting the molecular constants deduced from the e - and f -parity levels, or they can be directly obtained by fitting the $TV_e - TV_f$ differences for each level to a second-order polynomial. The results of both methods are presented in Sect. 3.5. Their values were graphically compared according to their oxygen isotopic content to check for anomalies that are due to perturbations. In almost every case, our molecular constants were generated by much larger datasets than those referenced in Sect. 2.1 (see also Table 2).

It is worth noting that the lines in the R - and P -branches are in general not observed up to the same J' . It is also possible, in the case of high-pressure spectra, that some lines observed at high J' values belong to a weak unidentified underlying band. As a consequence, some reduced term value graphs could present a break or jump for the last higher J' values. This break, however, could correspond in some cases to a real perturbation.

3. Results and discussion

The results presented here constitute the first part of an atlas of the Rydberg states at wavelengths below 115 nm for six isotopologues of CO. They update and complete the previous CO atlas at the higher resolution provided by the VUV-FTS coupled to the SOLEIL synchrotron (Eidelsberg et al. 1991; for revised band origin wavenumbers, see Eidelsberg et al. 1992). They also fill some gaps and provide higher J' lines that were previously not observed with high-resolution laser methods.

In addition to the atlas of absolute wavelengths and wavenumbers for the B , C , and E states of the six CO isotopologues, we provide for the derived term value atlas for each observed band. As a further step, we calculate reduced term values and molecular parameters. The latter are compared according to their oxygen isotopic content, and when possible, with previous determinations.

Figure 1 shows the bandhead wavelengths of the states and bands studied in this work. Table 1 summarizes the measured bands for each isotopologue. Some isotopologue bands are not recorded because of the combination of low oscillator strengths and low available pressures or partial pressures. Low partial pressure is particularly a problem in the case of $^{13}\text{C}^{17}\text{O}$, which is observed as a minor contaminant in high-pressure spectra of both $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$.

For all ^{12}C (or ^{13}C)-bearing isotopologues, the isotope shift spacing between bandheads increases almost linearly with v' vibrational number, allowing for an easier differentiation of the lines pertaining to a given isotopologue for increasing v' and J' .

3.1. Specific cases of $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$

3.1.1. $^{12}\text{C}^{17}\text{O}$

As $^{12}\text{C}^{17}\text{O}$ is mixed in almost equal proportions with $^{12}\text{C}^{16}\text{O}$ in our sample, the absolute calibration of $^{12}\text{C}^{17}\text{O}$ transitions benefits from the absolute calibration of $^{12}\text{C}^{16}\text{O}$ (as well as $^{12}\text{C}^{18}\text{O}$, which is also present in a small amount).

3.1.2. $^{13}\text{C}^{17}\text{O}$

The case of $^{13}\text{C}^{17}\text{O}$ is specific because it is observed in the high-pressure spectra of either $^{13}\text{C}^{16}\text{O}$ or $^{13}\text{C}^{18}\text{O}$. The occurrence of the $^{13}\text{C}^{17}\text{O}$ bands is due to isotopic contamination of the $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$ bottles. Based on the relative strengths of identical absorption features, the ratio of the isotopologues

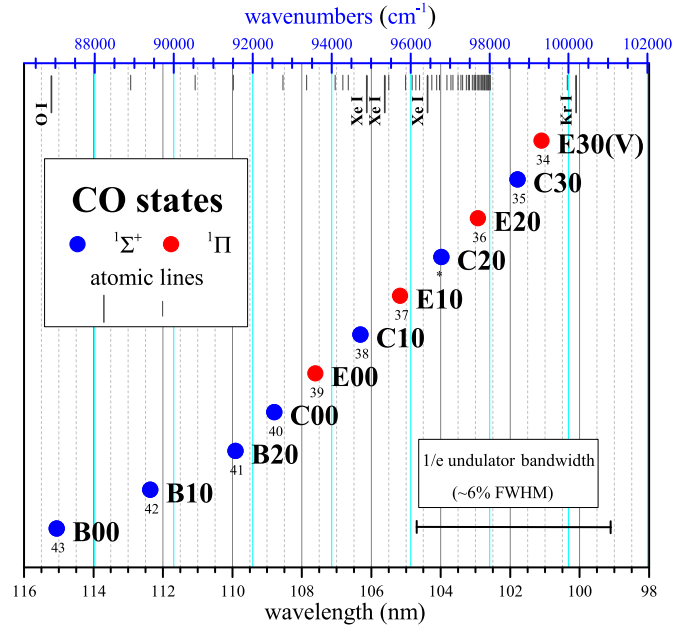


Fig. 1. Bandhead wavelengths of $^{12}\text{C}^{16}\text{O}$ states and bands studied in this work. We also include the previously used numerical index notation (34–43) (Letzelter et al. 1987; Eidelsberg & Rostas 1990, etc.). Atomic line calibrators are indicated with $|$ for primary lines at high accuracy (1 fm or better) and with $|$ for secondary lines at medium accuracy (0.1 pm) (for the latter, mostly Xe I and a few Ar I and Kr I, see the NIST atomic line tables for identification), and the $1/e$ undulator bandwidth are shown as well.

in the $^{13}\text{C}^{16}\text{O}$ gas sample, sorted by concentration, is found to be $^{13}\text{C}^{16}\text{O}:^{13}\text{C}^{18}\text{O}:^{13}\text{C}^{17}\text{O}:^{12}\text{C}^{16}\text{O} = 1:0.041:0.073:0:0045$. The high CO pressure needed to observe the minor $^{13}\text{C}^{17}\text{O}$ species leads to strong absorption and saturation of the main species spectrum. Combined with the fact that the isotopic shifts of $v' = 0$ bands are very small ($\leq 1 \text{ cm}^{-1}$ for B00 and C00 and $\leq 3 \text{ cm}^{-1}$ for E00), $^{13}\text{C}^{17}\text{O}$ lines for low J' are difficult to extract because of blending with saturated (broadened) lines. This effect is weaker for increasing J' because of the difference between molecular constants of the different isotopologues. $^{13}\text{C}^{17}\text{O}$ lines of B00 with $J' > 2$ are measured nearly as accurately ($\sim 0.04 \text{ cm}^{-1}$) as for the main isotopologue (either $^{13}\text{C}^{16}\text{O}$ or $^{13}\text{C}^{18}\text{O}$), similarly for C00 lines with $J' > 6$. The search for low J' line positions is facilitated by considering the values extrapolated from the clearly observed high J' line levels (up to $J' = 23$ for B00, $J' = 21$ for B10, $J' = 39$ for C10, and $J' = 26$ for E00), which leads to an accuracy better than 0.08 cm^{-1} for the low J' . This effect is less noticeable for $v' \geq 1$ as the spacing of spectra bandheads of the different isotopologues increases with v' .

All this concerns R - and P -branches, but there is an additional difficulty for Q -branches that we consider in the E -state subsection.

3.2. $X^1\Sigma^+$ state

In order to calculate the term values of all the bands presented here, high-accuracy data provided by Guelachvili et al. (1983) and Farrenq et al. (1991) were used. From their set of Dunham coefficients, rotational levels of the $v'' = 0$ $X^1\Sigma^+$ ground state were calculated up to $J'' = 48$ with an uncertainty of 10^{-3} cm^{-1} , which is at least as good as our own high-resolution measurements. Table 9 lists the ground-state rotational levels of the six

Table 3. References to table and figure numbers for the $B^1\Sigma^+$ state.

Band	Transition		Term values	Reduced TV
	wavelengths			
	Tables	Figure	Table	Figure
	^{12}C	^{13}C		
B00	A.1	A.2	2	A.3
B10	A.4	A.5	3	A.6
B20	A.7	A.7	A.1	A.8

isotopologues studied here, $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, and $^{13}\text{C}^{18}\text{O}$. For each isotopologue, these J'' levels are adjusted to a ninth-order polynomial to obtain their molecular constants. They are reported in Table A.31.

For the sake of consistency between all isotopologues, we did not use the data on the $^{12}\text{C}^{16}\text{O}$ ground state by Varberg & Evenson (February 1992), which were published a few months after Farrenq et al. (October 1991). The latter provide data for six isotopologues, and a check on $^{12}\text{C}^{16}\text{O}$ B00 revealed a better agreement at high J' between the term values TV_R and TV_P derived for the R - and P -branches.

3.3. $B^1\Sigma^+$ state

The B00 and B10 bands were observed for all isotopologues, while B20 was observed for all bands except for $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$. The lack of the B20 band in the $^{12}\text{C}^{17}\text{O}$ spectra is explained by the low pressure used in scans of this isotopologue. For $^{13}\text{C}^{17}\text{O}$, the absence is due to the combination of a very low partial pressure and the decreasing oscillator strength with ν' .

A total of 19 CO laser-calibrated lines (14 for $^{12}\text{C}^{16}\text{O}$, 2 for $^{12}\text{C}^{18}\text{O}$, and 3 for $^{13}\text{C}^{16}\text{O}$) were used to determine a shift correction of -7.5×10^{-6} nm (0.006 cm^{-1}) for B00 and 3 lines for B10, resulting in a shift correction of -1.2×10^{-5} nm (0.0095 cm^{-1}). These low values attest to the accuracy of our measurements. These corrections were applied to all isotopologues as their spectra are placed, as mentioned above, on a unique scale. Our term values are consistent within the uncertainty with those calculated by Le Floch & Amiot (1985) and Haridass et al. (1994), the latter resulting from the combination of B - A data with high-resolution A - X data obtained with the former Ottawa 10.6 m vacuum-grating spectrograph. For $^{12}\text{C}^{16}\text{O}$ B00, the average difference between our values and the Daprà et al. (2016) values is 5.0×10^{-6} nm.

For $^{12}\text{C}^{17}\text{O}$, the present results complete a preliminary version of our B00 data that was incorporated in Hakalla et al. (2016) in order to perform the deperturbation analysis of the $A^1\Pi$ state of $^{12}\text{C}^{17}\text{O}$, for which earlier optical measurements of B - A and C - A transitions were combined with our vacuum ultraviolet B - X results. Similarly, for $^{13}\text{C}^{17}\text{O}$, our results of B00 and B10 were used in Hakalla et al. (2017) to perform the deperturbation analysis of the $A^1\Pi$ state of $^{13}\text{C}^{17}\text{O}$.

The data for $^{13}\text{C}^{18}\text{O}$ are slightly better calibrated than in our recent paper (Lemaire et al. 2016) for B00 and B10. In addition, they are extended to higher J' levels for B10.

As indicated above, the B20 band was calibrated using the surrounding B10 and C00 bands, leading to a common shift correction of $+1.0 \times 10^{-5}$ nm (-0.0083 cm^{-1}) that was applied to all isotopologues. Figure A.3 illustrates for the four observed isotopologues the perturbations observed in B20 (also studied in $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ by Baker 1994).

Table 4. Statistical uncertainty on the measured term values: δ_P average and std. dev. (at 2σ) (see Sect. 2.2.2) for the $B^1\Sigma^+$ state.

Band	Species	N	$\overline{\delta_P}$ (cm^{-1})	Std. dev. (cm^{-1})
B00	1216	62	0.000	0.007
	1217	44	0.007	0.023
	1218	60	0.003	0.022
	1316	60	0.011	0.026
	1317	36	0.001	0.026
B10	1318	54	0.002	0.006
	1216	60	0.00	0.02
	1217	30	-0.010	0.033
	1218	52	-0.001	0.009
	1316	54	-0.001	0.013
B20	1317	40	-0.011	0.027
	1318	38	0.007	0.010
	1216	22	-0.003	0.034
	1217			
	1218	22	0.019	0.038
	1316	30	-0.006	0.021
	1317			
	1318	30	-0.005	0.032

Notes. N : number of rotational transitions (R and P) involved in the statistics.

For $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$, our absolutely calibrated data provide transition frequencies and term values for B00, B10, and B20 that are consistent at slightly higher accuracy with those measured by Eidelsberg et al. (1987), which were obtained with the Observatoire de Paris (Meudon, France) 10 m VUV grating spectrograph. The same remark applies to the line positions obtained by Baker (1994) for B20 of $^{12}\text{C}^{16}\text{O}$ with the same instrument.

Table 3 lists table and figure numbers associated with the BX bands. Table 4 gives the statistical uncertainty on the term values for the BX bands (see text in Sect. 2.2.2).

3.4. $C^1\Sigma^+$ state

C00, C10, C20, and C30 were observed for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$. For $^{12}\text{C}^{17}\text{O}$, all bands were observed except for C20, for the same reason as for B20. For $^{13}\text{C}^{17}\text{O}$, only C00 and C10 were observed; C20 and C30 are not observed for the same reason as for B20.

It is worth noting that for $^{12}\text{C}^{18}\text{O}$, the C30 band does not appear in the same room-temperature spectra obtained at pressures where C20 is observed. It is only observed in a low-temperature spectrum recorded at 90 ± 5 K, showing a limited number of J' levels.

Sixteen CO laser-calibrated lines were used to determine a shift correction of 1.3×10^{-5} nm (-0.011 cm^{-1}) for C00. Seventy-two laser-calibrated lines were considered (not including $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$, for which the number of lines in Cacciani et al. 2001 is limited) to determine the shift correction of 3.4×10^{-5} nm (-0.031 cm^{-1}) for C10.

Our term values are consistent with those calculated by Haridass et al. (1994), which were obtained from the combination of C - A data with high-resolution A - X data obtained with the former Ottawa spectrograph. For $^{12}\text{C}^{16}\text{O}$ C00, the average difference between our values and the values of Daprà et al. (2016) is 4.4×10^{-5} nm (-0.037 cm^{-1}).

For C00, the present results complete a preliminary version of our $^{12}\text{C}^{17}\text{O}$ data (as for B00) and provide new data on $^{13}\text{C}^{17}\text{O}$.

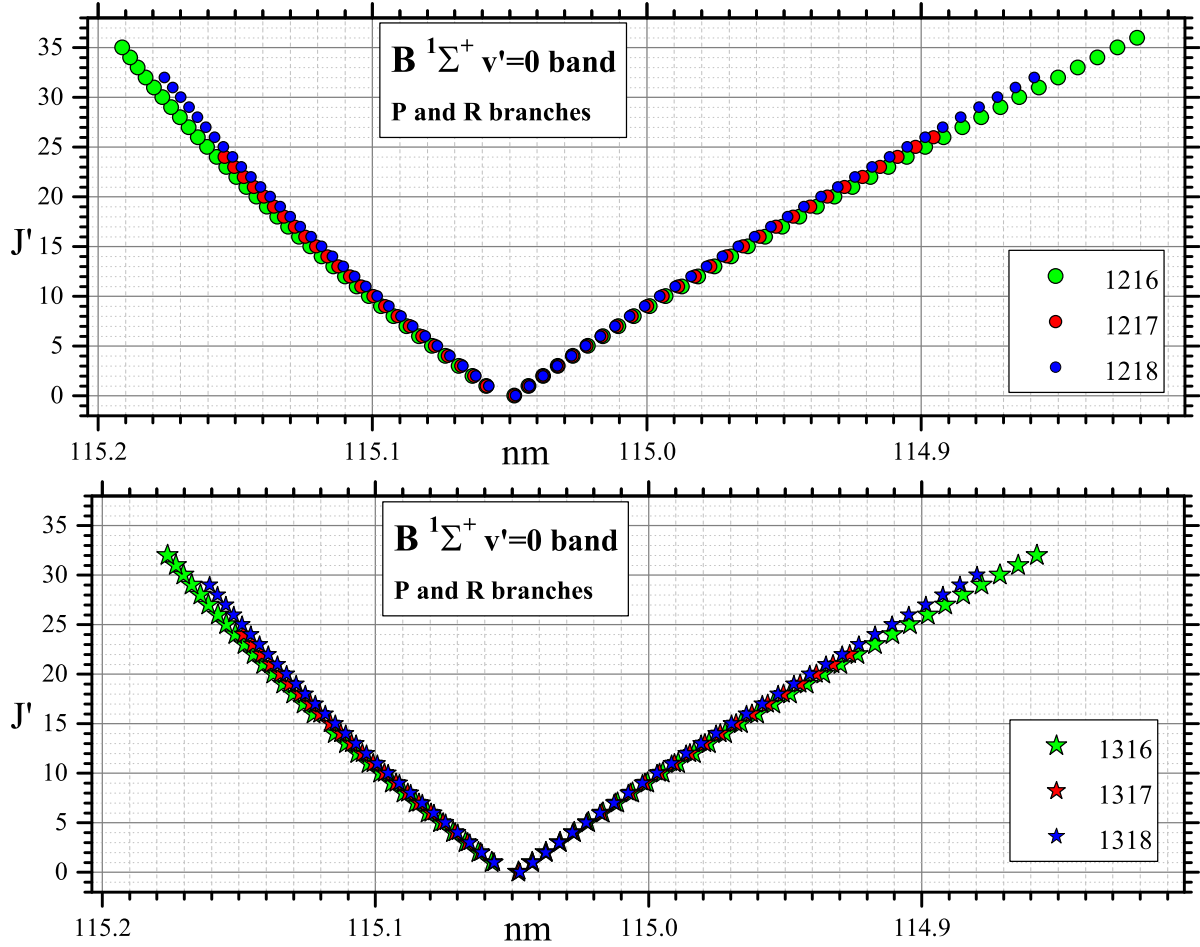


Fig. 2. Transition wavelengths of the $B^1\Sigma^+(v'=0)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

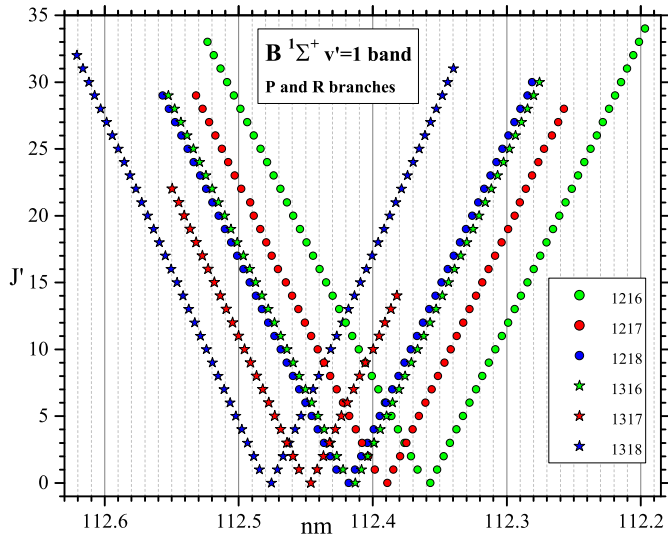


Fig. 3. Transition wavelengths of the $B^1\Sigma^+(v'=1)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

Both were used in order to perform the deperturbation analysis of the $A^1\Pi$ state of $^{12}\text{C}^{17}\text{O}$ (Hakalla et al. 2016) and of $^{13}\text{C}^{17}\text{O}$ (Hakalla et al. 2017).

As for B00 and B10, the present data for $^{13}\text{C}^{18}\text{O}$ are slightly better calibrated and extend to higher J' levels than in our recent paper (Lemaire et al. 2016) for C00.

Table 5. References to table and figure numbers for the $C^1\Sigma^+$ state.

Band	Transition wavelengths		Term values	Reduced TV	
	Figure			Table	Figure
	^{12}C	^{13}C			
C00	A.9	A.10	A.4	A.11	A.6
C10	A.12	A.13	A.5	A.14	A.7
C20	A.15	A.15	A.8	A.16	A.9
C30	A.17	A.17	A.10	A.18	A.11

The absolute calibration for C20 and C30 was obtained using the two surrounding primary atomic standards as calibrators (the Xe I line at 104.383497 nm for C20, and the Kr I line at 100.1060639 nm for C30, see Fig. 1) and checking that the numerous secondary standards (in the case of C20) are in agreement with each other (at an accuracy higher than 0.01 pm) for the five isotopologues.

Table 5 lists table and figure numbers associated with the CX bands. Table 6 gives the statistical uncertainty on the term values for the CX bands (see text in Sect. 2.2.2).

3.5. $E^1\Pi$ state

E00, E10, E20, and E30 [the latter formerly labeled as the $V(A^2\Pi)^3\Pi$ state by Eidelsberg & Rostas (1990), with the present assignment confirmed by Lefebvre-Brion & Eidelsberg (2012)] were observed for all isotopologues, with the exception

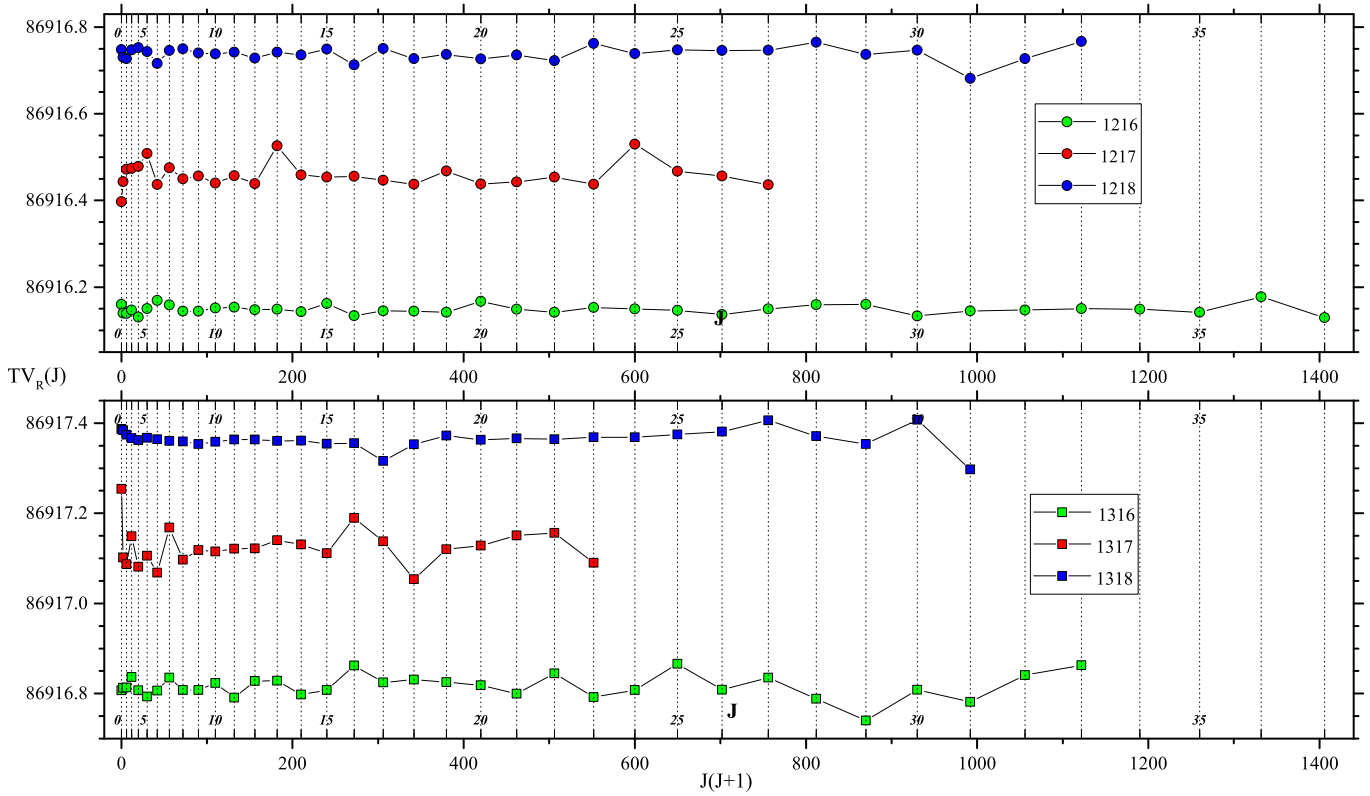


Fig. 4. Reduced term values (cm^{-1}) of the $B^1\Sigma^+(v'=0)$ levels for six CO isotopologues.

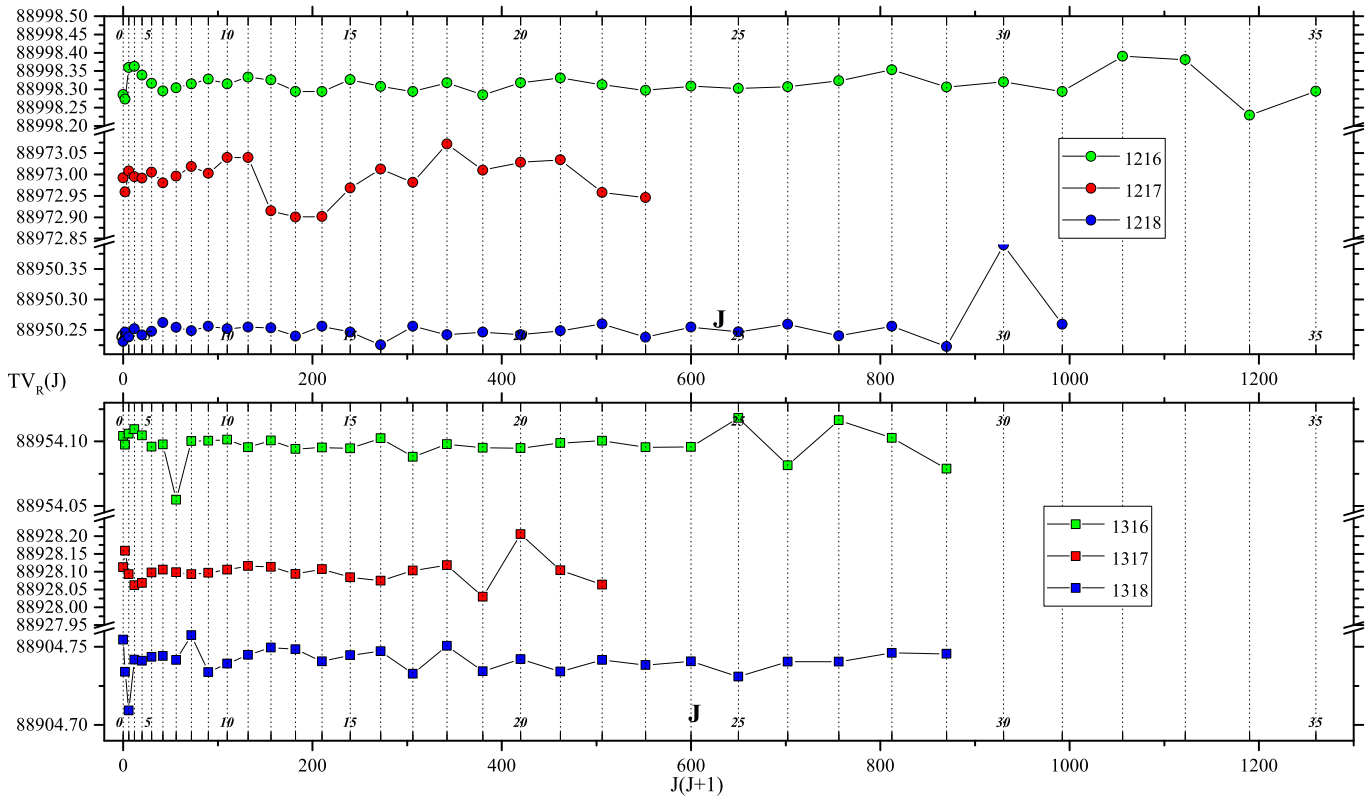


Fig. 5. Reduced term values (cm^{-1}) of the $B^1\Sigma^+(v'=1)$ levels for six CO isotopologues.

of E20 and E30 for $^{13}\text{C}^{17}\text{O}$ (as for B20 because of the combination of a very low partial pressure and decreasing oscillator strength with ν').

For E20 and E30 of $^{12}\text{C}^{18}\text{O}$, the same remark holds as for C30. These two bands do not appear in spectra taken at room-temperature at pressures where E10 is observed. It is only observed in low-temperature spectra recorded at 90 ± 5 K, showing a limited number of J' .

For all isotopologues, the rotational spacing is extremely small for the Q -branch of E00, E10, and E20, giving rise to congested spectra that require better resolution than available with the VUV-FTS and smaller Doppler broadening. This is particularly noticeable for the Q -branch of E10, where the lines are very slightly blueshifted with J' compared to the Q -branch of E00, which is slightly blueshifted, and the Q -branch of E20, which is slightly redshifted. Only with the use of a very narrow-band laser were Cacciani & Ubachs (2004) able to separate the Q -branch of E00, and Ubachs et al. (2000) did this in combination with a deperturbation analysis for E10. The Q -branch of E30 has a very different aspect (similar to $A-X$ transitions) with a redshifted Q -branch and a returning limb for the R -branch with increasing J' (see for comparison Figs. A.12, A.17, and A.25 vs. A.28, and also Figs. A.15, A.16, A.24, and A.27 vs. Figs. A.30–A.36).

A careful analysis is required to distinguish the lines in the E00 bands of the different isotopologues. Spectra recorded at different pressures were used for this purpose. Figure A.16 illustrates the difficulty of this task for E00 with three spectra for $^{13}\text{C}^{18}\text{O}$ and 2 for $^{13}\text{C}^{16}\text{O}$. Figure A.27 shows the easier example of E20 for $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$, and Figs. A.30–A.36 show the example of E30 for $^{13}\text{C}^{18}\text{O}$.

There is very good agreement for the R - and P -branch line positions between our present results and other high-resolution measurements (Cacciani et al. 1995; Cacciani & Ubachs 2004 for E00 and Ubachs et al. 2000 for E10).

E00 was calibrated using a few levels observed by Cacciani et al. (1995) for $^{12}\text{C}^{16}\text{O}$ [3 lines] and a large set of R and P levels (Cacciani & Ubachs 2004) for $^{12}\text{C}^{16}\text{O}$ [60 lines] and $^{13}\text{C}^{16}\text{O}$ [32 lines] obtained by their methods labeled 1 and 0 (these data have to be calculated from the supplementary data, but no data are available for $^{13}\text{C}^{18}\text{O}$). The resulting shift correction is estimated as 2.3×10^{-5} nm (-0.020 cm $^{-1}$). Comparison to Daprà et al. (2016) shows an average difference of 3.8×10^{-5} nm for E00. For $^{12}\text{C}^{18}\text{O}$ and $^{13}\text{C}^{18}\text{O}$, our term values for E00 (e - and f -parity) match those calculated by Haridass et al. (1994) well, which were obtained from the combination of $E-A$ data with high-resolution $A-X$ data collected with the former Ottawa spectrograph. For the Q -branch of $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$, which we cannot separate, we report the Cacciani & Ubachs (2004) observed transition frequencies (see their Table 1). We merged the Cacciani et al. data with our higher- J' measurements. For the other isotopologues, $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$, the Q bandhead up to $J' \approx 9$ was simulated to reproduce the observed spectra. These calculated data were merged with our measured data at higher J' . For the last isotopologue, $^{13}\text{C}^{17}\text{O}$, the Q -branch was simulated by interpolation of the $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$ transitions (but these data are not reported in the table) in order to assign the few observed high J' Q -lines.

E10 was calibrated by a few lines observed by Cacciani et al. (1995) for $^{12}\text{C}^{16}\text{O}$ [9 lines] and a large set by Ubachs et al. (2000) of R and P lines for $^{12}\text{C}^{16}\text{O}$ [42 R and P lines], for $^{12}\text{C}^{17}\text{O}$ [2 R lines], $^{12}\text{C}^{18}\text{O}$ [24 P and R lines], $^{13}\text{C}^{16}\text{O}$ [25 P and R lines], and $^{13}\text{C}^{18}\text{O}$ [18 R lines]. The absolute calibration for E10 obtained with the R and P levels is also confirmed by the presence of closely surrounding Xe I atomic lines (see Fig. 1).

Table 6. Statistical uncertainty on the measured term values: δ_P average and std. dev. (at 2σ) (see Sect. 2.2.2) for the $C^1\Sigma^+$ state.

Band	Species	N	$\overline{\delta_P}$ (cm $^{-1}$)	Std. dev. (cm $^{-1}$)
C00	1216	72	0.010	0.027
	1217	66	-0.011	0.034
	1218	70	0.000	0.010
	1316	72	0.000	0.013
	1317	70	0.004	0.021
	1318	78	-0.001	0.007
C10	1216	62	0.001	0.013
	1217	42	0.001	0.010
	1218	52	-0.008	0.022
	1316	54	0.008	0.045
	1317	44	0.006	0.043
	1318	56	-0.003	0.017
C20	1216	28	0.003	0.012
	1217			
	1218	14	0.007	0.044
	1316	16	0.004	0.043
	1317			
	1318	14	-0.015	0.019
C30	1216	32	0.025	0.038
	1217	6	-0.007	0.048
	1218	16	-0.002	0.053
	1316	16	-0.004	0.056
	1317			
	1318	26	0.016	0.044

Notes. N : number of rotational transitions (R and P) involved in the statistics.

The resulting shift correction is estimated to be 5.0×10^{-6} nm. As it is not possible to distinguish the Q -branch of E10 for all isotopologues, we report in the tables the values obtained by Ubachs et al. (2000), merged with our measured data at higher J' . Our dataset for R - and P -branches extends those of Ubachs et al. (2000) to high J' values. Sample spectra are shown for $^{12}\text{C}^{16}\text{O}$ in Fig. A.20, $^{12}\text{C}^{17}\text{O}$ in Fig. A.21, $^{12}\text{C}^{18}\text{O}$ in Fig. A.22, $^{13}\text{C}^{16}\text{O}$ in Fig. A.23, and $^{13}\text{C}^{18}\text{O}$ in Fig. A.24. All of them show additional lines, and among them, lines that belong to the perturbing state $k^3\Pi(\nu' = 5$ and $6) - X^1\Sigma^+(\nu' = 0)$ (Baker & Launay 1994; Ubachs et al. 2000). The lower panel of Fig. A.21 shows the simulated absorption spectrum of $^{12}\text{C}^{17}\text{O}$ at room temperature.

For E20 and E30, only low-resolution spectra without absolute calibration are available (Ogawa & Ogawa 1974 for $^{12}\text{C}^{16}\text{O}$ E20) and the Eidelsberg et al. (1991) atlas for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ for both E20 and E30, with either measured or extrapolated or calculated line positions. Consequently, the absolute calibration of E20 and E30, for which there are no previous high-resolution measurements, was obtained in the same way as for C20 and C30, using the two surrounding primary atomic standards as calibrators and checking that the numerous secondary standards (in the case of E20) are in agreement with each other (at an accuracy higher than 0.01 pm) for five isotopologues (with the exception of $^{13}\text{C}^{17}\text{O}$). For E20, the Q -branch up to $J' = 6$ or 7 was obtained in the same way as for E10 by simulating our recorded spectra and merging them with the higher measurable J' , up to ~ 10 – 20 , depending on the isotopologue. Figure A.27 shows the simulated absorption spectra of $^{12}\text{C}^{16}\text{O}$ at 90 K and at room temperature. Finally, as indicated above, all branches of E30 have well-resolved transitions for all observed

Table 7. References to table and figure numbers for the $E^1\Pi$ state.

Band	Transition wavelengths		Term values		Reduced TV	
	Tables		Table	Figure		
	^{12}C	^{13}C		e -par.	f -par.	
E00	A.19	A.20	A.12	A.21	A.13	A.14
E10	A.22	A.23	A.17	A.24	A.18	A.19
E20	A.25	A.26	A.25	A.29	A.26	
E30	A.27	A.28	A.28	A.30	A.29	

isotopologues. Figures A.30–A.36 show spectra for all five isotopologues; in some cases, the results obtained at 293 K and 90 K are compared, which are useful to separate the R -branch lines.

In order to verify the quality of our frequency determinations for the Q -branch, we use a method similar to the combination differences. We compared the values of the Λ -type doubling of the upper state obtained through the R - and P -branches, $\Lambda_R(J)$ and $\Lambda_P(J)$ (for $J \geq 1$) with

$$\Lambda_R(J) = [R(J-1) + X(J-1)] - [Q(J) + X(J)] \text{ and}$$

$$\Lambda_P(J) = [P(J+1) + X(J+1)] - [Q(J) + X(J)].$$

For all isotopologues and all bands (E00, E01, E02, and E03), the results are consistent with the value of Λ_d provided in the term value tables. The Λ doubling of the upper state is graphically represented for all isotopologues in each band, E00, E10, E20, and E30, in Fig. A.37 together with polynomial fits (linear in most cases).

Table 7 lists table and figure numbers associated with the EX bands. Table 8 gives the statistical uncertainty on the e -parity term values of the EX bands (see text in Sect. 2.2.2).

4. Concluding remarks

Our work presents a comprehensive and homogeneous set of absolutely calibrated line positions from which term values and molecular constants are derived. In most cases, these were obtained from larger sets of data than earlier determinations. Our data complete previous determinations and fill many gaps, particularly concerning the B20, C20, C30, E20, and E30 bands of all isotopologues. We also provide new data, particularly for the $^{12}\text{C}^{17}\text{O}$ and $^{13}\text{C}^{17}\text{O}$ isotopologues.

A final verification of the absolute accuracy of our whole set of results is provided by comparison with the data reported by Daprà et al. (2016). These datasets were not considered as calibrators because they were derived from others cited in Sect. 2.1, but we verified that they are in good agreement (at least for the six J' levels included therein) with our own results on B00, C00, and E00 for $^{12}\text{C}^{16}\text{O}$.

In conclusion, the overall uncertainty of our data is a combination of the relative fitting accuracy in line positions (for a well-resolved typical line $\sim 0.008 \text{ cm}^{-1}$) and of the accuracy in the calibrators and in the ground state (up to $\sim 0.003 \text{ cm}^{-1}$). Most of the line positions are thus determined to an accuracy of $\sim 0.009 \text{ cm}^{-1}$. For some weak (mainly at high J') or a few blended lines, the fitting errors are estimated to be as large as $0.10\text{--}0.15 \text{ cm}^{-1}$. Uncertainties on term value data are reflected in the δ_P values presented in the term value tables.

Molecular constants are compiled in Table A.31 for all states and bands. In this table the E state e - and f -parity are treated independently, and we calculate in Table A.32 $T_v(1)$ (average of

Table 8. Statistical uncertainty on the measured term values: δ_P average and std. dev. (at 2σ) (see Sect. 2.2.2) for the e -parity levels (R and P) for the $E^1\Pi$ state.

Band	Species	N	$\overline{\delta_P}$ (cm^{-1})	Std. dev. (cm^{-1})
E00	1216	58	0.002	0.014
	1217	48	0.003	0.015
	1218	64	0.001	0.014
	1316	74	0.009	0.018
	1317	30	-0.008	0.018
	1318	68	0.018	0.032
E10	1216	50	0.004	0.031
	1217	38	0.009	0.024
	1218	44	0.004	0.021
	1316	54	0.000	0.018
	1317	36	-0.001	0.002
	1318	62	0.009	0.026
E20	1216	36	0.003	0.015
	1217	18	-0.004	0.026
	1218	20	0.008	0.015
	1316	36	0.001	0.014
	1317			
	1318	48	-0.003	0.027
E30	1216	30	-0.001	0.046
	1217	16	-0.002	0.037
	1218	18	-0.005	0.030
	1316	18	0.003	0.019
	1317			
	1318	22	0.000	0.010

Notes. N : number of rotational transitions (R and P) involved in the statistics.

T_v for e - and f -parity), $q_v = B_e - B_f$, and $q_{Dv} = D_e - D_f$. These molecular constants are also obtained by a quadratic fit of the Λ -doubling data shown in Fig. A.37 and reported in Table A.33.

In order to check the consistency of our term values, we compare their trends for the six CO isotopologues in Fig. A.38. The term value differences between ^{16}O and ^{18}O bearing isotopologues are compared both for ^{12}C and ^{13}C versus the B , C , and E states. Term values are also compared as a function of v' for each states, and a linear fit is drawn through all isotopologues present in each (T_v, v') data point. Both comparisons show a similar behavior.

The statistical table for the term values (see Tables 4, 6, and 8) can reveal the possible presence of perturbations when there is a large spread in the standard deviation ($>0.043 \text{ cm}^{-1}$, namely for $^{12}\text{C}^{16}\text{O}$ (E30), for $^{12}\text{C}^{17}\text{O}$ (C30), for $^{12}\text{C}^{18}\text{O}$ (C20 and C30), for $^{13}\text{C}^{16}\text{O}$ (C10, C20 and C30), for $^{13}\text{C}^{17}\text{O}$ (C10), and for $^{13}\text{C}^{18}\text{O}$ (C30). Anomalies in the molecular constants also reveal evidence of perturbations, as shown in Fig. A.39, which illustrates this point more clearly than Table A.31. While T_v mainly depends on the absolute calibration, B_v and especially D_v are very sensitive to perturbations, as shown in Fig. A.39.

Perturbations will be discussed in detail in a subsequent paper. Another forthcoming development of this work will be a comprehensive atlas of oscillator strengths and cross sections for the states, bands, and isotopologues presented here.

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Table 9. Rotational energy levels (cm^{-1}) of the $X^1\Sigma^+$ ground state for six CO isotopologues (calculated from the Farrenq et al. 1991 Dunham coefficients).

J''	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	0	0	0	0	0	0
1	3.845	3.748	3.662	3.676	3.579	3.493
2	11.535	11.244	10.986	11.028	10.736	10.478
3	23.069	22.487	21.971	22.055	21.472	20.956
4	38.448	37.477	36.617	36.757	35.786	34.926
5	57.670	56.214	54.924	55.134	53.677	52.388
6	80.735	78.696	76.891	77.185	75.145	73.340
7	107.642	104.924	102.518	102.909	100.190	97.783
8	138.390	134.895	131.802	132.305	128.809	125.715
9	172.978	168.610	164.743	165.372	161.003	157.136
10	211.404	206.066	201.341	202.109	196.770	192.044
11	253.667	247.262	241.593	242.515	236.108	230.438
12	299.766	292.197	285.498	286.588	279.017	272.317
13	349.698	340.869	333.055	334.326	325.495	317.679
14	403.461	393.276	384.261	385.727	375.540	366.523
15	461.054	449.416	439.116	440.791	429.150	418.847
16	522.475	509.288	497.616	499.515	486.324	474.650
17	587.721	572.888	559.761	561.896	547.059	533.928
18	656.789	640.215	625.546	627.932	611.354	596.681
19	729.677	711.266	694.971	697.622	679.206	662.906
20	806.383	786.039	768.033	770.962	750.612	732.601
21	886.902	864.530	844.729	847.950	825.571	805.763
22	971.233	946.737	925.056	928.582	904.079	882.391
23	1059.372	1032.657	1009.011	1012.857	986.133	962.480
24	1151.315	1122.285	1096.591	1100.771	1071.731	1046.028
25	1247.059	1215.620	1187.794	1192.320	1160.870	1133.034
26	1346.601	1312.658	1282.615	1287.502	1253.546	1223.492
27	1449.936	1413.395	1381.051	1386.312	1349.757	1317.401
28	1557.061	1517.827	1483.099	1488.748	1449.498	1414.757
29	1667.971	1625.950	1588.755	1594.805	1552.767	1515.557
30	1782.662	1737.760	1698.015	1704.480	1659.559	1619.797
31	1901.131	1853.254	1810.876	1817.769	1769.870	1727.473
32	2023.371	1972.426	1927.332	1934.667	1883.698	1838.582
33	2149.380	2095.273	2047.380	2055.170	2001.037	1953.120
34	2279.151	2221.790	2171.015	2179.274	2121.884	2071.084
35	2412.680	2351.972	2298.233	2306.975	2246.234	2192.468
36	2549.962	2485.814	2429.030	2438.267	2374.083	2317.268
37	2690.991	2623.311	2563.400	2573.145	2505.427	2445.482
38	2835.763	2764.459	2701.339	2711.606	2640.260	2577.102
39	2984.271	2909.251	2842.841	2853.643	2778.577	2712.127
40	3136.509	3057.682	2987.901	2999.252	2920.375	2850.549
41	3292.473	3209.748	3136.515	3148.427	3065.647	2992.366
42	3452.156	3365.442	3288.676	3301.163	3214.389	3137.572
43	3615.552	3524.758	3444.380	3457.454	3366.596	3286.161
44	3782.655	3687.690	3603.619	3617.295	3522.261	3438.129
45	3953.457	3854.233	3766.390	3780.679	3681.380	3593.470
46	4127.954	4024.380	3932.685	3947.601	3843.946	3752.179
47	4306.137	4198.125	4102.499	4118.054	4009.954	3914.251
48	4488.001	4375.461	4275.825	4292.033	4179.399	4079.679

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Appendix A: Additional figures and tables

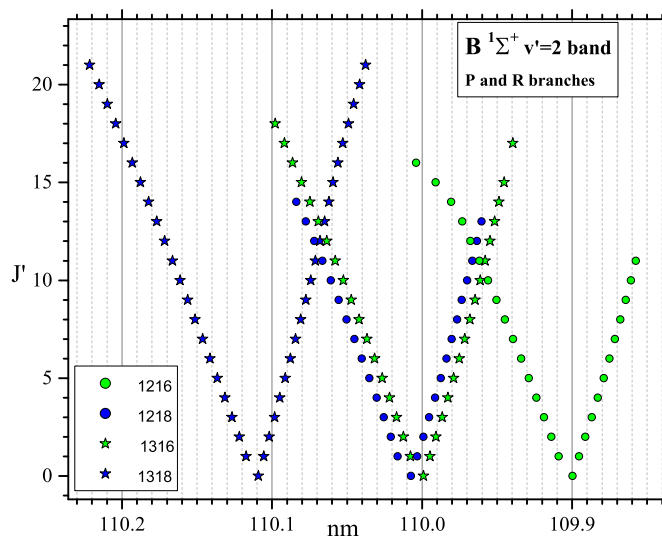


Fig. A.1. Transition wavelengths of the $B^1\Sigma^+(v'=2)-X^1\Sigma^+(v''=0)$ band for the four observed CO isotopologues.

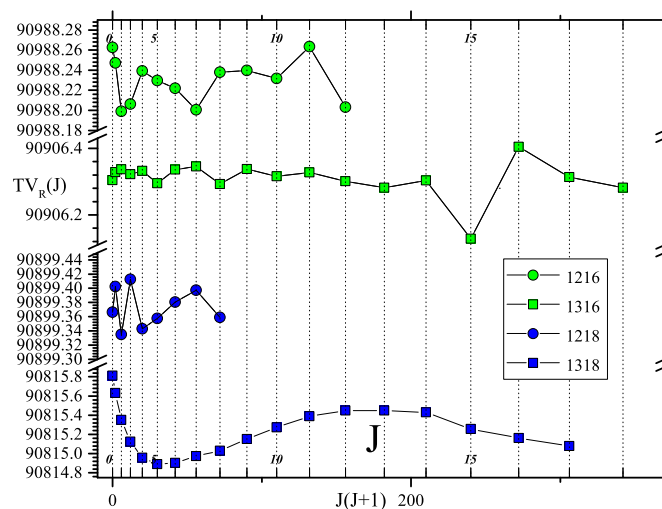


Fig. A.2. Reduced term values (cm^{-1}) of the $B^1\Sigma^+(v'=2)$ levels for the four observed CO isotopologues.

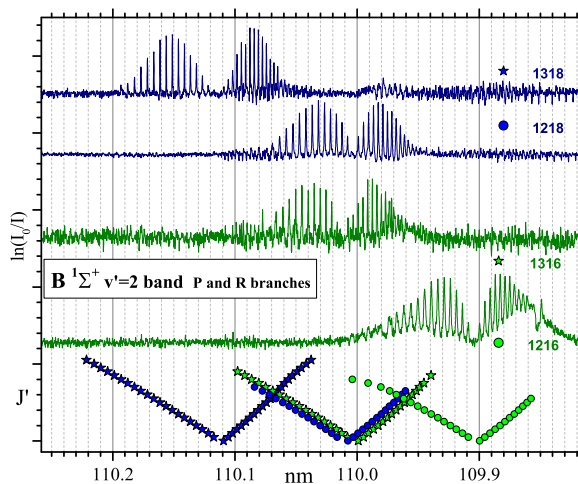


Fig. A.3. Sample of B20 spectra for the four observed isotopologues, in some cases showing perturbations.

Table A.1. Measured transition wavelengths and wavenumbers of the $B^1\Sigma^+(v''=0)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, and $^{12}\text{C}^{18}\text{O}$.

J''	$^{12}\text{C}^{16}\text{O}$				$^{12}\text{C}^{17}\text{O}$				$^{12}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	δP
0	115.04826	115.05849	86920.042	6	115.04802	115.05805	86920.225	-17	115.04772	115.05747	86920.452	10
1	115.04305	115.06355	86923.984	1	115.04289	115.06286	86924.101	-17	115.04274	115.06229	86924.214	16
2	115.03774	115.06850	86927.998	9	115.03770	115.06765	86928.023	5	115.03766	115.06702	86931.892	26
3	115.03240	115.07339	86932.031	9	115.03245	115.07244	86931.990	20	115.03258	115.07166	86935.799	3
4	115.02696	115.07823	86936.140	0	115.02708	115.07715	86936.048	51	115.02744	115.07621	86939.706	14
5	115.02144	115.08294	86940.314	6	115.02189	115.08178	86939.971	0	115.02224	115.08076	86943.750	-4
6	115.01590	115.08766	86944.501	3	115.01641	115.08637	86944.113	9	115.01689	115.08523	86947.780	9
7	115.01030	115.09233	86948.737	4	115.01098	115.09103	86948.218	11	115.01156	115.08960	86951.870	-15
8	115.00463	115.09709	86953.021	3	114.99982	115.09527	86952.437	16	115.00067	115.09389	86956.013	-11
9	114.99887	115.10125	86957.379	-12	114.99844	115.10083	86956.656	16	114.99514	115.10237	86960.195	-9
10	114.99304	115.10565	86961.787	-8	114.99412	115.10396	86960.966	17	114.98953	115.10648	86964.437	-21
11	114.98716	115.11000	86966.228	3	114.98844	115.10818	86965.262	-5	114.98382	115.11059	86968.756	20
12	114.98121	115.11428	86970.730	2	114.98244	115.11233	86974.081	63	114.97812	115.11460	86973.067	10
13	114.97524	115.11849	86975.249	9	114.97678	115.11640	86978.566	-17	114.97233	115.11853	86977.447	2
14	114.96914	115.12261	86979.863	-8	114.97085	115.12041	86983.090	-2	114.96654	115.12237	86981.828	-1
15	114.96304	115.12666	86984.475	1	114.96487	115.12440	86987.654	6	114.96062	115.12622	86990.824	-23
16	114.95686	115.13070	86989.151	-17	114.95884	115.12830	86992.241	8	114.95465	115.12988	86995.373	10
17	114.95060	115.13459	86993.892	-7	114.95278	115.13215	86996.913	-23	114.94864	115.13363	86999.959	-4
18	114.94430	115.13846	86998.662	9	114.94661	115.13590	87001.608	2	114.94258	115.13721	87004.607	-3
19	114.93770	115.14226	87003.527	-8	114.94040	115.13954	87006.349	-5	114.93027	115.14077	87009.278	0
20	114.93149	115.14597	87008.359	-7	114.93414	115.14325	87011.143	-8	114.92399	115.14424	87014.032	-9
21	114.92501	115.14963	87013.265	3	114.92781	115.14680	87016.015	51	114.91774	115.15097	87018.765	-18
22	114.91843	115.15323	87018.241	-3	114.92137	115.15028	87020.926	16	114.91137	115.15428	87023.589	16
23	114.91184	115.15676	87023.231	2	114.91489	115.15382	87025.775	1	114.90494	115.15751	87028.458	-9
24	114.90519	115.16021	87028.271	-6	114.90849	115.15732	87030.716	1	114.89851	115.16071	87033.329	16
25	114.89849	115.16360	87033.342	2	114.90196	115.16071	87035.688	1	114.89198	115.16379	87038.275	-1
26	114.89170	115.16694	87038.490	6	114.89540	115.16379	87043.673	6	114.88544	115.16681	87048.216	18
27	114.88486	115.17019	87043.673	9	114.88954	115.16681	87048.216	-10	114.87886	115.16985	87053.300	99
28	114.87798	115.17337	87048.886	0	114.89196	115.16985	87053.300	0	114.86552	115.17272	87058.325	99
29	114.87110	115.17650	87054.100	6	114.89540	115.17272	87063.479	0	114.85872	115.17581	87068.325	99
30	114.86409	115.17958	87059.409	2	114.89954	115.17581	87068.325	0				
31	114.85707	115.18257	87064.733	9	114.89304	115.17886	87073.716	6				
32	114.84998	115.18550	87070.105	6	114.88716	115.18257	87079.044	0				
33	114.84285	115.18848	87075.509	6	114.88121	115.18550	87084.459	0				
34	114.83569	115.19146	87080.944	2	114.87524	115.18848	87090.426	0				
35	114.82841	115.19444	87086.459	2	114.86914	115.19146	87096.493	0				
36	114.82121	115.19742	87091.926	2	114.86304	115.19444	87102.509	0				

Notes. Column description (refer also to Sect. 2.2) for each isotopologue. Col. 1: J'' . Cols. 2 and 3: R_c and P_c calibrated wavenumbers. Col. 4: δP wavenumber corrections applied to TV_P in units of the least significant digit ($-\delta P$ is applied to TV_P). No value indicates the absence of one of the branches, either R or P . An asterisk indicates when both R - and P -branches are present at high J'' , either the potential presence of a perturbing state or that one of the lines shows a larger uncertainty than the other.

Table A.2. Measured transition wavelengths and wavenumbers of the $B^1\Sigma^+(\nu''=0)-X^1\Sigma^+(\nu''=0)$ band for $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δP
0	115.04759	115.05741	86920.550	86913.131	115.04746	115.05669	86920.648	-80	115.04708	115.05640	86920.935	11
1	115.04260	115.06222	86924.320	86909.498	115.04250	115.06146	86924.396	9	115.04236	115.06098	86924.501	1
2	115.03751	115.06695	86928.166	86905.925	115.03741	115.06261	86928.242	72	115.03756	115.06548	86928.128	3
3	115.03243	115.07159	86932.005	86902.421	115.03261	115.07076	86931.869	0	115.03269	115.06993	86931.809	3
4	115.02726	115.07623	86935.912	86898.917	115.02753	115.07524	86935.708	-1	115.02777	115.07432	86935.527	9
5	115.02199	115.08079	86939.895	86895.474	115.02247	115.07963	86939.533	0	115.02278	115.07861	86939.298	-4
6	115.01664	115.08525	86943.939	86892.106	115.01717	115.08404	86943.539	-2	115.01773	115.08287	86943.115	0
7	115.01130	115.08962	86947.976	86888.807	115.01206	115.08820	86947.402	16	115.01262	115.08707	86946.978	4
8	115.00586	115.09398	86952.089	86885.500	115.00669	115.09250	86951.462	2	115.00746	115.08707	86950.879	6
9	115.00033	115.09828	86956.270	86882.269	115.00136	115.09669	86955.491	-22	115.00224	115.09120	86954.826	5
10	114.99480	115.10248	86960.452	86879.099	114.99597	115.09669	86959.567	8	114.99694	115.09257	86958.834	-7
11	114.98919	115.10668	86964.695	86875.929	114.99049	115.10078	86963.711	-17	114.99160	115.10319	86962.872	-1
12	114.98340	115.11065	86969.074	86872.933	114.98491	115.10478	86967.932	0	114.98619	115.10706	86966.963	-6
13	114.97778	115.11477	86973.325	86869.824	114.97932	115.10876	86972.160	8	114.98074	115.11089	86971.086	3
14	114.97190	115.11868	86977.773	86866.876	114.97368	115.11267	86976.426	18	114.97520	115.11463	86975.276	-6
15	114.96607	115.12261	86982.183	86863.908	114.96798	115.11654	86980.738	-68	114.96964	115.11836	86979.482	18
16	114.96015	115.12625	86986.663	86861.161	114.96218	115.12036	86985.127	7	114.96406	115.12197	86983.704	5
17	114.95415	115.13010	86991.203	86858.257	114.95640	115.12386	86989.500	54	114.95832	115.12559	86988.047	7
18	114.94813	115.13379	86995.759	86855.473	114.95050	115.12768	86993.965	-2	114.95255	115.12905	86992.414	10
19	114.94202	115.13741	87000.383	86852.742	114.94454	115.13144	86998.476	1	114.94678	115.13585	86996.780	13
20	114.93588	115.14100	87005.031	86849.372	114.93845	115.13480	87003.085	45	114.94092	115.14242	87001.216	2
21	114.92967	115.14453	87009.732	86847.875	114.93244	115.13825	87007.635	1	114.92907	115.14561	87005.674	6
22	114.92345	115.14784	87014.441	86842.266	114.92641	115.14167	87012.200	2	114.92305	115.14876	87010.186	-3
23	114.91707	115.15130	87019.272	86839.762	115.14828				114.91699	115.15182	87014.744	-4
24	114.91069	115.15462	87024.104	86837.432					114.91087	115.15483	87019.333	5
25	114.90421	115.15771	87029.011	86835.883					114.90468	115.15775	87023.967	-2
26	114.89776	115.16109	87033.897	86830.261					114.89849	115.16072	87028.655	-2
27	114.89128	115.16410	87038.806	86827.969					114.89227	115.16259	87033.344	-6
28	114.88477	115.16722	87043.738	86825.813					114.88589	115.16594	87038.056	13
29	114.87802	115.17026	87048.852	86823.589					114.87968		87042.889	
30	114.87132	115.17312	87053.929								87047.594	
31	114.86461	115.17607	87059.015									
32	114.85780	115.17907	87064.177									

Table A.3. Term values (cm^{-1}) of the $B^1\Sigma^+(v'=0)$ levels for six CO isotopologues.

J'	$B^1\Sigma^+(v'=0)$					
	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	86916.160	86916.397	86916.748	86916.807	86917.254	86917.387
1	86920.036 (6)	86920.242 (−17)	86920.441 (10)	86920.538 (12)	86920.728 (−80)	86920.924 (11)
2	86927.828 (1)	86927.866 (−17)	86927.860 (16)	86927.988 (8)	86927.965 (9)	86927.993 (1)
3	86939.524 (9)	86939.261 (5)	86939.012 (26)	86939.186 (8)	86938.906 (72)	86938.604 (3)
4	86955.091 (9)	86954.456 (20)	86953.860 (3)	86954.056 (4)	86953.341 (0)	86952.756 (9)
5	86974.588 (0)	86973.474 (51)	86972.402 (14)	86972.664 (5)	86971.495 (−1)	86970.457 (−4)
6	86997.979 (6)	86996.185 (0)	86994.635 (−4)	86995.022 (7)	86993.210 (0)	86991.686 (0)
7	87025.233 (3)	87022.801 (9)	87020.633 (9)	87021.118 (6)	87018.686 (−2)	87016.452 (4)
8	87056.375 (4)	87053.147 (−5)	87050.312 (−15)	87050.879 (6)	87047.613 (−22)	87044.756 (6)
9	87091.422 (−12)	87087.316 (16)	87083.682 (−11)	87084.386 (8)	87080.255 (16)	87076.590 (5)
10	87130.365 (−8)	87125.255 (11)	87120.766 (−9)	87121.628 (14)	87116.492 (2)	87111.969 (−7)
11	87173.190 (2)	87167.015 (17)	87161.557 (−21)	87162.539 (22)	87156.359 (−22)	87150.879 (−1)
12	87219.893 (3)	87212.529 (−5)	87206.032 (−1)	87207.234 (−25)	87199.837 (−17)	87193.316 (−6)
13	87270.486 (9)	87261.933 (63)	87254.234 (20)	87255.606 (55)	87246.948 (0)	87239.278 (3)
14	87324.954 (−8)	87314.967 (−17)	87306.112 (10)	87307.659 (−9)	87297.646 (8)	87288.771 (−6)
15	87383.326 (−2)	87371.844 (−2)	87361.707 (2)	87363.461 (39)	87351.948 (18)	87341.782 (18)
16	87445.528 (1)	87432.507 (−1)	87420.944 (−1)	87423.016 (−41)	87409.956 (−68)	87398.324 (5)
17	87511.644 (−17)	87496.935 (6)	87483.946 (−23)	87486.183 (−6)	87471.444 (7)	87458.347 (7)
18	87581.619 (−7)	87565.139 (−9)	87550.575 (10)	87553.097 (2)	87536.506 (54)	87521.965 (10)
19	87655.461 (−10)	87637.152 (−23)	87620.923 (−4)	87623.698 (−6)	87605.321 (−2)	87589.082 (13)
20	87733.196 (9)	87712.873 (2)	87694.934 (−3)	87697.994 (11)	87677.680 (1)	87659.685 (2)
21	87814.750 (−8)	87792.393 (−5)	87772.643 (−3)	87775.973 (19)	87753.653 (45)	87733.811 (6)
22	87900.174 (−7)	87875.682 (−8)	87854.007 (0)	87857.707 (−25)	87833.204 (1)	87811.440 (−3)
23	87989.471 (3)	87962.700 (51)	87939.097 (−9)	87943.030 (−6)	87916.277 (2)	87892.581 (−4)
24	88082.606 (−3)	88053.582	88027.794 (−18)	88032.105 (24)		87977.219 (5)
25	88179.588 (−2)	88148.060	88120.189 (−9)	88124.904 (−30)		88065.363 (−2)
26	88280.407 (−6)	88246.337	88216.236 (16)	88221.263 (68)		88157.003 (−2)
27	88385.089 (2)	88348.346	88315.945 (−1)	88321.380 (18)		88252.153 (−6)
28	88493.603 (6)		88419.326 (1)	88425.092 (26)		88350.732 (13)
29	88605.938 (9)		88526.311 (18)	88532.467 (18)		88452.813
30	88722.072 (−1)		88636.981 (−10)	88643.620 (38)		88558.446
31	88842.065 (6)		88751.216 (99)	88758.333 (77)		88667.391
32	88965.864 (0)		88869.201	88876.784		
33	89093.476		88990.811	88998.843		
34	89224.889					
35	89360.095					
36	89499.139					
37	89641.888					

Notes. The δ_P value in parentheses (in units of the least significant digit) corresponds to the wavenumber correction applied to TV_P and TV_R . There is no value when the term value is derived from a single transition, either R or P . An asterisk indicates when both R - and P -branches are present at high J' , either the potential presence of a perturbing state or that one of the lines shows a larger uncertainty than the other (see also Sect. 2.2.2).

Table A.4. Transition wavelengths and wavenumbers of the $B^1\Sigma^+(\nu' = 1) - X^1\Sigma^+(\nu'' = 0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, and $^{12}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{12}\text{C}^{16}\text{O}$				$^{12}\text{C}^{17}\text{O}$				$^{12}\text{C}^{18}\text{O}$				
	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (cm $^{-1}$)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δp
0	112.35693	112.36657	89002.078	-39	112.38895	112.39839	88976.717	12	112.41779	112.42705	88953.892	88946.569	-17
1	112.35196	112.37139	89006.010	-36	112.38419	112.40319	88980.487	12	112.41315	112.43163	88957.565	88942.939	2
2	112.34707	112.37614	89009.885	-5	112.37947	112.40783	88984.226	-13	112.40851	112.43630	88961.238	88939.252	-1
3	112.34225	112.38104	89013.704	-2	112.37475	112.41260	88987.965	-4	112.40389	112.44090	88964.891	88935.609	-1
4	112.33743	112.38593	89017.523	8	112.36999	112.41734	88991.734	-5	112.39925	112.44554	88968.564	88931.939	5
5	112.33261	112.39083	89021.342	2	112.36530	112.42208	88995.443	9	112.39461	112.45017	88972.240	88928.281	4
6	112.32779	112.39572	89025.162	7	112.36054	112.42685	88999.214	4	112.39000	112.45477	88975.886	88924.639	4
7	112.32290	112.40055	89029.037	-16	112.35582	112.43159	89002.959	21	112.38538	112.45940	88979.547	88920.982	-3
8	112.31809	112.40544	89032.856	19	112.35113	112.43629	89006.668	7	112.38075	112.46404	88983.209	88917.313	0
9	112.31327	112.41027	89036.675	-1	112.34637	112.44103	89010.440	-3	112.37615	112.46865	88986.856	88913.669	-5
10	112.30845	112.41517	89040.494	9	112.34165	112.44573	89014.181	5	112.36692	112.47327	88994.166	88910.015	0
11	112.30363	112.42007	89044.313	-8	112.33723	112.45047	89017.688	-96	112.36232	112.47789	88997.804	88906.360	0
12	112.29889	112.42489	89048.076	5	112.33246	112.45523	89021.460	-41	112.35772	112.48252	89001.453	88902.705	3
13	112.29407	112.42979	89051.895	-9	112.32778	112.46005	89025.172	-41	112.35309	112.48716	89005.116	88899.035	-9
14	112.28926	112.43469	89055.714	8	112.32291	112.46475	89029.034	-63	112.34856	112.49175	89008.710	88895.409	24
15	112.28451	112.43952	89059.477	-2	112.31811	112.46947	89032.839	0	112.34397	112.49643	89012.345	88891.714	2
16	112.27977	112.44442	89063.240	-9	112.31335	112.47416	89036.613	28	112.33938	112.50105	89015.982	88888.060	-24
17	112.27495	112.44932	89067.059	-14	112.30844	112.47900	89040.502	100	112.33479	112.50560	89019.617	88884.462	2
18	112.27021	112.45421	89070.822	9	112.30364	112.48367	89044.308	*	112.33025	112.51028	89023.214	88880.767	15
19	112.26547	112.45919	89074.585	41	112.29881	112.48861	89048.141	*	112.32572	112.51492	89026.808	88877.101	4
20	112.26080	112.46402	89078.292	16	112.29409	112.49337	89051.886	*	112.32116	112.51955	89030.416	88873.449	-12
21	112.25605	112.46885	89082.055	-33	112.28929	112.49804	89055.692	*	112.31664	112.52415	89033.999	88869.811	-12
22	112.25138	112.47368	89085.762	16	112.28449	112.50297	89059.499	*	112.31213	112.52878	89037.580	88866.158	5
23	112.24671	112.47851	89089.469	17	112.28000	112.50773	89063.305	*	112.30764	112.53347	89041.137	88862.453	-8
24	112.24204	112.48334	89093.175	5	112.27551				112.30314	112.53808	89044.704	88858.814	-11
25	112.23744	112.48817	89096.826	25	112.27102				112.29867	112.54274	89048.246	88855.135	-13
26	112.23277	112.49300	89100.533	-7	112.26653				112.29421	112.54738	89051.787	88851.472	5
27	112.22818	112.49783	89104.183	20	112.26204				112.28981	112.55209	89055.274	88847.753	-2
28	112.22365	112.50266	89107.778	-4	112.25755				112.28532				
29	112.21912	112.50749	89111.372	9	112.25306				112.28083				
30	112.21467	112.51232	89114.911	-19	112.24857				112.27634				
31	112.21014	112.51715	89118.505	-44	112.24408				112.27185				
32	112.20554	112.52198	89122.156	*	112.23959				112.26736				
33	112.20130	112.52681	89125.826		112.23510				112.26287				
34	112.19682	112.53164	89129.089		112.23061				112.25838				

Table A.5. Transition wavelengths and wavenumbers of the $B^1\Sigma^+(\nu' = 1) - X^1\Sigma^+(\nu'' = 0)$ band for $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$						
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δp
0	112.41288	112.4217	88957.775	88950.428	2	112.44578	112.45491	88931.752	88924.534	14	112.47553	112.48434	88908.224	88901.262	-4
1	112.40823	112.42682	88961.460	88946.745	1	112.44134	112.45939	88935.259	88920.988	7	112.47108	112.48078	88911.748	88897.755	47
2	112.40358	112.43146	88965.140	88943.079	1	112.43684	112.46399	88938.822	88917.351	21	112.46667	112.49329	88915.235	88894.190	4
3	112.39895	112.43610	88968.803	88939.408	-8	112.43232	112.46857	88942.395	88913.731	8	112.46224	112.49761	88918.736	88890.780	6
4	112.39430	112.44074	88972.484	88935.739	6	112.42778	112.47307	88945.987	88910.174	-10	112.45781	112.50202	88922.237	88887.293	4
5	112.38966	112.44541	88976.160	88932.044	4	112.42326	112.47753	88949.566	88906.648	-19	112.45339	112.50642	88925.731	88883.815	-5
6	112.38508	112.45005	88979.784	88928.376	-3	112.41872	112.48203	88953.154	88903.091	-3	112.44896	112.51081	88929.232	88880.345	-4
7	112.38038	112.45473	88983.506	88924.670	0	112.41420	112.48657	88956.732	88899.498	0	112.44452	112.51522	88932.750	88876.865	-5
8	112.37574	112.45932	88987.179	88921.043	2	112.40967	112.49110	88960.317	88895.920	2	112.44011	112.51960	88936.232	88873.407	-2
9	112.37111	112.46396	88990.843	88917.372	-5	112.40515	112.49562	88963.898	88892.353	-4	112.43566	112.52403	88939.751	88869.908	9
10	112.36648	112.46859	88994.512	88913.710	3	112.40061	112.50011	88967.491	88888.802	0	112.43124	112.52843	88943.255	88866.432	4
11	112.36184	112.47325	88998.185	88910.028	6	112.39606	112.50461	88971.089	88885.244	23	112.42680	112.53281	88946.766	88862.974	9
12	112.35724	112.47789	89001.833	88906.362	0	112.39159	112.50915	88974.629	88881.657	6	112.42239	112.53720	88950.256	88859.508	-1
13	112.35261	112.48253	89005.499	88902.694	7	112.38708	112.51366	88978.199	88878.094	-13	112.41797	112.54158	88953.752	88856.052	4
14	112.34802	112.48718	89009.138	88899.019	-6	112.38259	112.51813	88981.753	88874.569	-10	112.41355	112.54598	88957.250	88852.576	1
15	112.34340	112.49181	89012.793	88895.363	-7	112.37807	112.52266	88985.332	88870.989	4	112.40912	112.55035	88960.754	88849.121	9
16	112.33882	112.49644	89016.428	88891.703	-1	112.37356	112.52719	88988.903	88867.414	-25	112.40472	112.55474	88964.233	88845.655	11
17	112.33422	112.50111	89020.070	88888.012	-6	112.36910	112.53161	88992.439	88863.923	-75	112.40031	112.55915	88967.723	88842.179	-4
18	112.32964	112.50574	89023.699	88884.355	-3	112.36466	112.53601	88995.953	88860.443	-42	112.39593	112.56349	88971.194	88838.754	-1
19	112.32506	112.51040	89027.330	88880.676	5	112.36016	112.54065	88999.520	88856.779	-16	112.39152	112.56790	88974.684	88835.276	3
20	112.32050	112.51506	89030.942	88876.993	-2	112.35553	112.54611	89003.189	88849.754	-82	112.38714	112.57227	88978.149	88831.822	2
21	112.31595	112.51970	89034.552	88873.325	0	112.35116	112.54955	89006.647	88846.247	-82	112.38275	112.57666	88981.624	88828.356	2
22	112.31141	112.52436	89038.146	88869.645	2	112.34666	112.55399				112.37839	112.58104	88985.082	88824.905	1
23	112.30689	112.52904	89041.731	88865.954	0						112.37402	112.58543	88991.979	88821.442	4
24	112.30237	112.53370	89045.313	88862.268	-16						112.36968	112.58982	88995.424	88817.981	3
25	112.29790	112.53833	89048.863	88858.615	7						112.36533	112.59422	88998.859	88814.508	0
26	112.29334	112.54309	89052.475	88854.858	31						112.36099	112.59859	89002.272	88811.056	6
27	112.28900	112.54776	89055.917	88851.165	-51						112.35668	112.60300	89005.666	88807.582	-6
28	112.28453	112.55238	89059.467	88847.525							112.35240	112.60738	89009.072	88804.129	-21
29	112.27983		89063.191								112.34810	112.61177	89012.434	88800.668	-45
30											112.34386	112.61611	89015.745	88797.245	-26
31															
32															

Table A.6. Term values (cm^{-1}) of the $B^1\Sigma^+(v' = 1)$ levels for six CO isotopologues.

J'	$B^1\Sigma^+(v' = 1)$					
	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	88998.285	88972.992	88950.231	88954.104	88928.113	88904.754
1	89002.117 (−39)	88976.706 (12)	88953.908 (−17)	88957.774 (2)	88931.738 (14)	88908.229 (−4)
2	89009.891 (−36)	88984.248 (−13)	88961.225 (2)	88965.135 (1)	88938.830 (7)	88915.193 (47)
3	89021.425 (−5)	88995.474 (−4)	88972.225 (−1)	88976.167 (1)	88949.538 (21)	88925.709 (4)
4	89036.776 (−2)	89010.457 (−5)	88986.863 (−1)	88990.866 (−8)	88963.859 (8)	88939.686 (6)
5	89055.970 (2)	89029.202 (9)	89005.177 (5)	89009.235 (6)	88981.783 (−10)	88957.159 (4)
6	89079.006 (7)	89051.653 (4)	89027.160 (4)	89031.290 (4)	89003.262 (−19)	88978.124 (−5)
7	89105.913 (−16)	89077.889 (21)	89052.781 (−3)	89056.972 (−3)	89028.303 (−3)	89002.576 (−4)
8	89136.660 (19)	89107.875 (7)	89082.060 (4)	89086.415 (0)	89056.922 (0)	89030.538 (−5)
9	89171.247 (−1)	89141.567 (−3)	89115.010 (0)	89119.482 (2)	89089.125 (2)	89061.950 (−2)
10	89209.644 (9)	89179.052 (−3)	89151.604 (−5)	89156.220 (−5)	89124.906 (−4)	89096.879 (9)
11	89251.906 (−8)	89220.242 (5)	89191.858	89196.619 (3)	89164.261 (0)	89135.295 (4)
12	89297.976 (5)	89265.046 (−96)	89235.759 (0)	89240.694 (6)	89207.174 (23)	89177.195 (9)
13	89347.851 (−9)	89313.698 (−41)	89283.299 (3)	89288.421 (0)	89253.640 (6)	89222.574 (−1)
14	89401.585 (8)	89366.104 (−63)	89334.517 (−9)	89339.818 (7)	89303.706 (−13)	89271.427 (4)
15	89459.177 (−2)	89422.310 (0)	89389.354 (24)	89394.872 (−6)	89357.303 (−10)	89323.772 (1)
16	89520.541 (−9)	89482.227 (28)	89447.823 (2)	89453.591 (−7)	89414.478 (4)	89379.593 (9)
17	89585.729 (−14)	89545.800 (100)	89509.985 (−24)	89515.943 (−1)	89475.252 (−25)	89438.872 (11)
18	89654.772 (9)	89613.225 (*)	89575.740 (2)	89581.971 (−6)	89539.574 (−75)	89501.656 (−4)
19	89727.571 (41)	89684.226 (*)	89645.149 (15)	89651.635 (−3)	89607.349 (−42)	89567.876 (−1)
20	89804.246 (16)	89759.033 (*)	89718.182 (4)	89724.947 (5)	89678.726	89637.588 (3)
21	89884.708 (−33)	89837.552 (*)	89794.854 (−12)	89801.906 (−2)	89753.817 (−16)	89710.749 (2)
22	89968.942 (16)	89919.709 (*)	89875.157 (−12)	89882.502 (0)	89832.299 (−82)	89787.386 (2)
23	90056.978 (17)	90005.651 (*)	89959.050 (5)	89966.726 (2)		89867.472 (1)
24	90148.835 (5)		90046.599 (−8)	90054.588 (0)		89951.018 (4)
25	90244.465 (25)		90137.739 (−11)	90146.100 (−16)		90038.004 (3)
26	90343.893 (−7)		90232.510 (−13)	90241.177 (7)		90128.457 (0)
27	90447.113 (20)		90330.857 (5)	90339.945 (31)		90222.345 (6)
28	90554.124 (−4)		90432.841 (−2)	90442.280 (−51)		90319.679 (−6)
29	90664.829 (9)		90538.373	90548.215		90420.444 (−21)
30	90779.363 (−19)			90657.996		90524.674 (−45)
31	90897.617 (−44)		90760.318			90632.256 (−26)
32	91019.750 (114)					90743.218
33	91145.527					
34	91274.905					
35	91408.240					

Notes. See note to Table A.3.

Table A.7. Transition wavelengths and wavenumbers of the $B^1\Sigma^+(\nu' = 2) - X^1\Sigma^+(\nu'' = 0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{12}\text{C}^{16}\text{O}$				$^{12}\text{C}^{17}\text{O}$				$^{12}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P
0	109.89971	109.92874	90992.051	56	109.98016	110.04008	90922.523	2	110.00738	110.01622	90902.992	39
1	109.89540	109.91868	90995.619	24	109.97346	110.05558	90931.030	42	110.00327	110.02077	90906.389	29
2	109.89111	109.92366	90999.172	17	109.96986	110.06082	90934.007	-63	109.99911	110.02550	90909.826	7
3	109.88689	109.92874	91002.666	22	109.96646	110.06633	90936.818	46	109.99518	110.03015	90913.075	31
4	109.88291	109.93391	91005.963	-34	109.96346	110.07184	90939.299	90	109.99130	110.03514	90916.282	14
5	109.87893	109.93930	91009.259	2	109.96049	110.07739	90941.838	*	109.98750	110.04008	90919.423	14
6	109.87509	109.94480	91012.440	26	109.95739	110.08381	90945.177	*	109.98375	110.04511	90922.523	2
7	109.87134	109.95028	91015.546	5	109.95431	110.08978	90948.666	*	109.98016	110.05028	90925.491	28
8	109.86773	109.95591	91018.537	-10	109.95177	110.09578	90952.152	*	109.97668	110.05558	90928.368	42
9	109.86416	109.96172	91021.494	33	109.94901	110.10178	90955.395	-37	109.97346	110.06082	90931.030	-13
10	109.86082	109.96739	91024.261	-75	109.94617	110.10784	90958.605	*	109.96986	110.06633	90934.007	-63
11	109.85751	109.97343	91027.004	-41	109.94332	110.11394	90961.818	*	109.96646	110.07184	90936.818	46
12					109.94049	110.12004	90965.049	*	109.96346	110.07739	90939.299	90
13					109.93768	110.12614	90968.282	*	109.96049	110.08381	90941.838	*
14					109.93487	110.13224	90971.515	*	109.95739	110.09036	90945.177	*
15					109.93206	110.13834	90974.748	*	109.95431	110.09691	90948.666	*
16					109.92925	110.14444	90977.981	*	109.95177	110.10346	90952.152	*
17					109.92644	110.15054	90981.214	*	109.94901	110.11001	90955.395	-37
18					109.92363	110.15664	90984.447	*	109.94617	110.11656	90958.605	*
19					109.92082	110.16274	90987.680	*	109.94332	110.12311	90961.818	*
20					109.91801	110.16884	90990.913	*	109.94049	110.12966	90965.049	*
21					109.91520	110.17494	90994.146	*	109.93768	110.13621	90968.282	*

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δ_P
%0	109.99898	109.99934	90909.934	19	110.10911	110.11722	90819.007	-15	110.10911	110.11722	90819.007	-15
1	109.99477	109.913413	90913.413	-9	110.10544	110.12178	90824.954	2	110.10544	110.12178	90824.954	2
2	109.99069	109.916786	90916.786	-32	110.09829	110.12662	90827.932	-39	110.09829	110.12662	90827.932	-39
3	109.98662	109.923358	90923.358	0	110.09475	110.13145	90830.853	11	110.09475	110.13145	90830.853	11
4	109.98274	109.926557	90926.557	7	110.09121	110.13643	90833.773	0	110.09121	110.13643	90833.773	0
5	109.97887	109.93168	90929.649	10	110.08767	110.14133	90836.694	-7	110.08767	110.14133	90836.694	-7
6	109.97513	109.93671	90932.568	18	110.08427	110.14624	90839.500	12	110.08427	110.14624	90839.500	12
7	109.97160	109.94188	90935.487	-6	110.08086	110.15121	90842.314	2	110.08086	110.15121	90842.314	2
8	109.96807	109.94718	90938.357	-13	110.07753	110.15625	90845.062	2	110.07753	110.15625	90845.062	2
9	109.96460	109.95242	90941.160	-53	110.07426	110.16130	90847.760	-5	110.07426	110.16130	90847.760	-5
10	109.96121	109.95793	90943.865	-13	110.07106	110.16641	90850.402	-7	110.07106	110.16641	90850.402	-7
11	109.95794	109.96344	90946.536	-5	110.06807	110.17159	90852.870	21	110.06807	110.17159	90852.870	21
12	109.95471	109.96907	90949.133	4	110.06501	110.17691	90855.395	-37	110.06501	110.17691	90855.395	-37
13	109.95157	109.97477	90951.524	30	110.06230	110.18223	90857.632	-10	110.06230	110.18223	90857.632	-10
14	109.94868	109.98041	90954.312	-9	110.05929	110.18768	90860.117	-10	110.05929	110.18768	90860.117	-10
15	109.94531	109.98638	90957.185	-11	110.05610	110.19314	90862.751	*	110.05610	110.19314	90862.751	*
16				-29	110.05283	110.19866	90865.451	-84	110.05283	110.19866	90865.451	-84
17	109.93942	110.09183	90959.185	90833.264	110.04901	110.20425	90868.605	59	110.04901	110.20425	90868.605	59
18				90828.328	110.04562	110.20978	90871.404	*	110.04562	110.20978	90871.404	*
19					110.04167	110.21522	90874.666	*	110.04167	110.21522	90874.666	*
20					110.03767	110.22149	90877.969	*	110.03767	110.22149	90877.969	*
21												

Table A.8. Term values (cm^{-1}) of the $B^1\Sigma^+(v'=2)$ levels for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$.

J'	$B^1\Sigma^+(v'=2)$					
	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	90988.263		90899.350	90906.304		90815.811
1	90991.994 (56)		90902.953 (39)	90909.915 (19)		90819.021 (-15)
2	90999.441 (24)		90910.021 (29)	90917.098 (-9)		90825.525 (2)
3	91010.690 (17)		90920.805 (7)	90927.845 (-32)		90835.471 (-39)
4	91025.714 (22)		90935.014 (31)	90942.205 (0)		90848.877 (11)
5	91044.445 (-34)		90952.885 (14)	90960.108 (7)		90865.779 (0)
6	91066.928 (2)		90974.345 (2)	90981.681 (10)		90886.168 (-7)
7	91093.150 (26)		90999.386 (28)	91006.816 (18)		90910.023 (12)
8	91123.183 (5)		91027.966 (42)	91035.483 (-6)		90937.280 (2)
9	91156.937 (-10)		91060.182 (-13)	91067.845 (-53)		90968.026 (2)
10	91194.439 (33)		91095.836 (-63)	91103.742 (-13)		91002.203 (-5)
11	91235.740 (-75)		91135.302 (46)	91143.274 (-5)		91039.811 (-7)
12	91280.712 (-41)		91178.322 (90)	91186.375 (4)		91080.819 (21)
13			91224.469 (*)	91233.094 (30)		91125.223 (-37)
14	91382.486		91274.893	91283.468 (-9)		91173.085 (-10)
15	91439.170			91337.262 (-11)		91224.278 (122)
16	91499.886			91395.131 (-29)		91279.049 (-84)
17				91456.260		91337.342 (59)
18				91521.080		91399.167 (*)
19						91464.729 (*)
20						91533.242 (*)
21						91607.267
22						91683.733

Notes. See note to Table A.3.

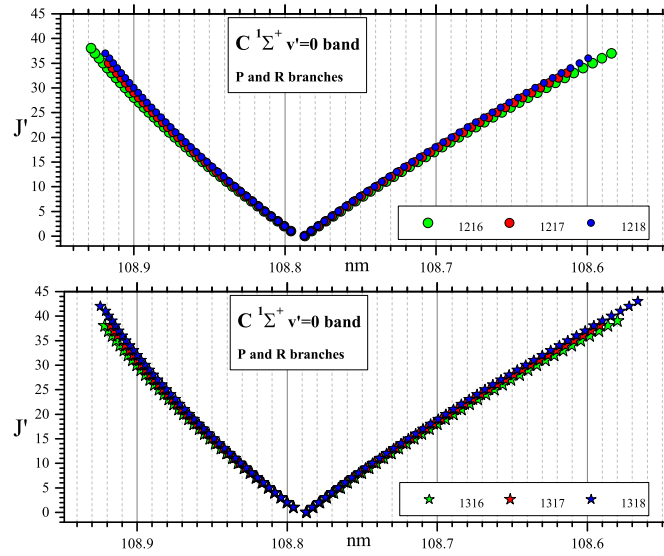


Fig. A.4. Transition wavelengths of the $C^1\Sigma^+(v'=0)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

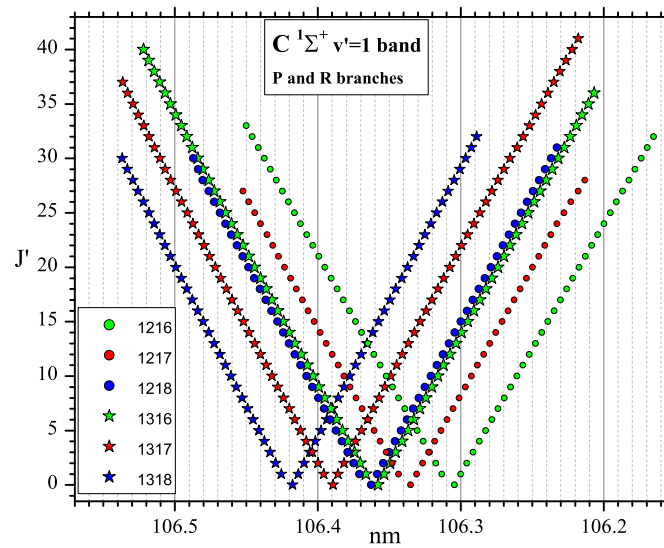


Fig. A.5. Transition wavelengths of the $C^1\Sigma^+(v'=1)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

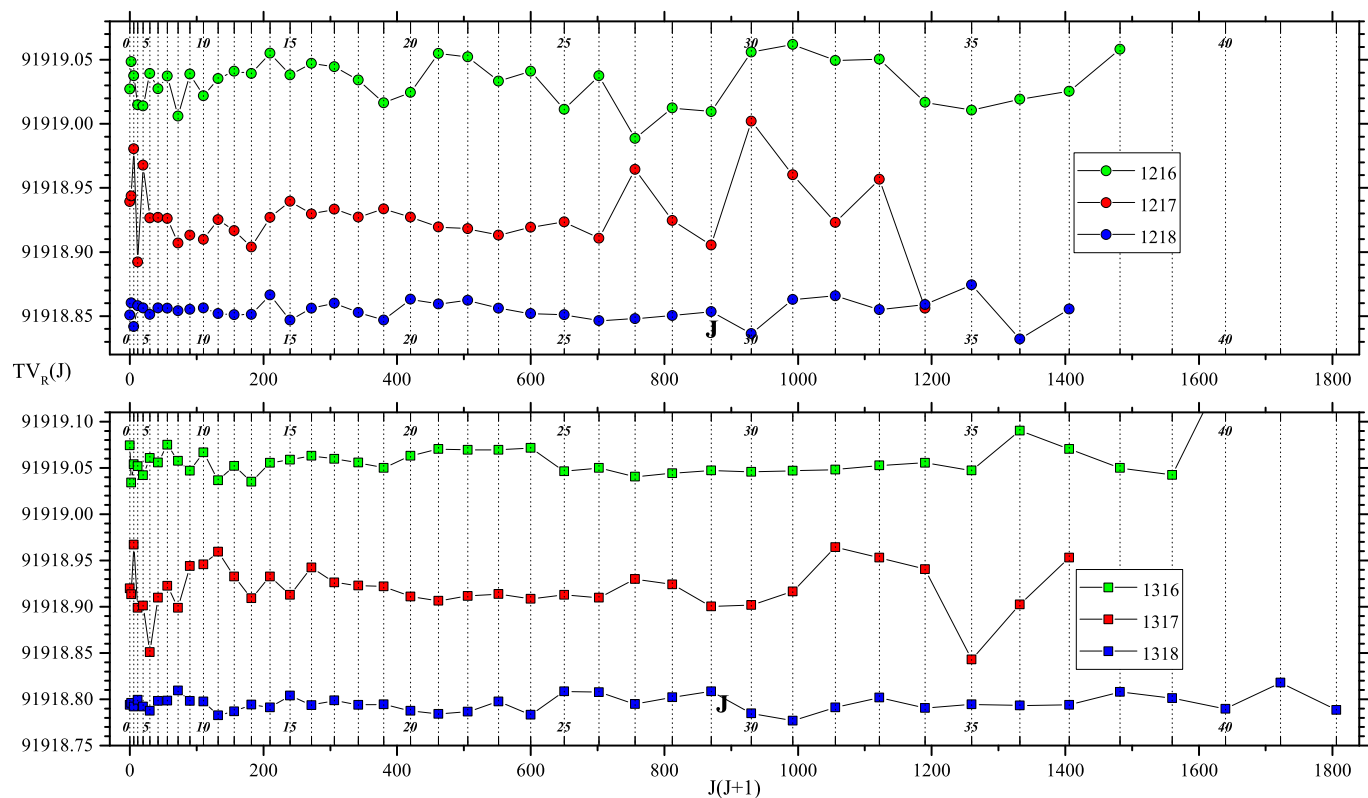


Fig. A.6. Reduced term values (cm^{-1}) of the $C^1\Sigma^+(v'=0)$ levels for six CO isotopologues.

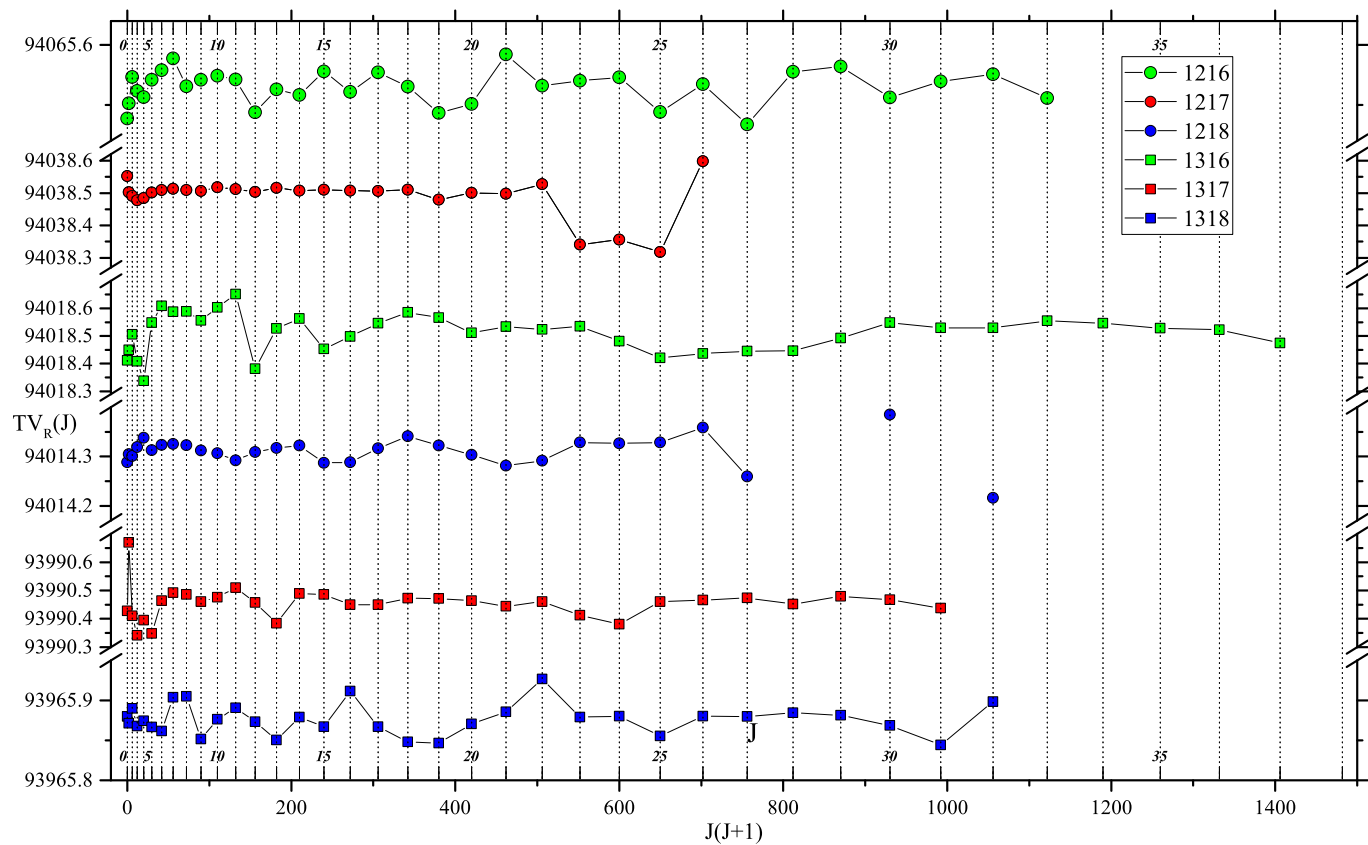


Fig. A.7. Reduced term values (cm^{-1}) of the $C^1\Sigma^+(v'=1)$ levels for six CO isotopologues.

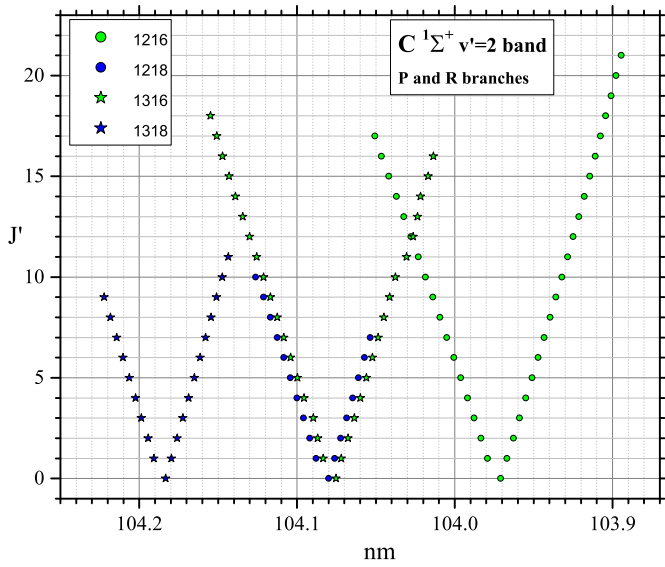


Fig. A.8. Transition wavelengths of the $C^1\Sigma^+(v'=2)-X^1\Sigma^+(v''=0)$ band for the four observed CO isotopologues.

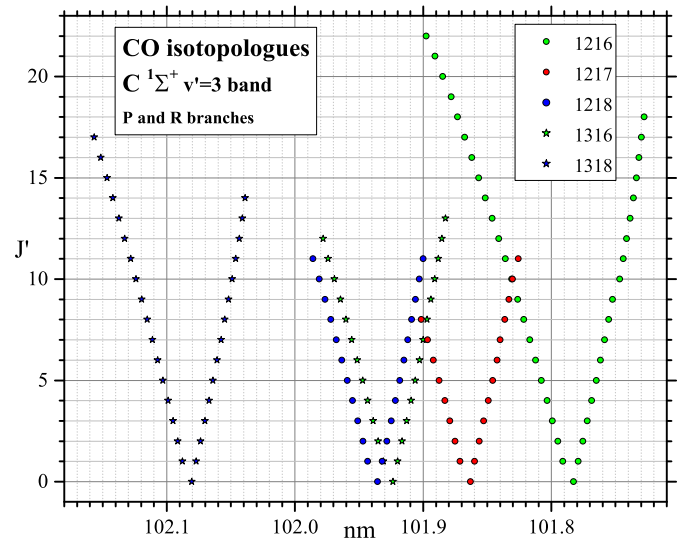


Fig. A.10. Transition wavelengths of the $C^1\Sigma^+(v'=3)-X^1\Sigma^+(v''=0)$ band for the five observed CO isotopologues.

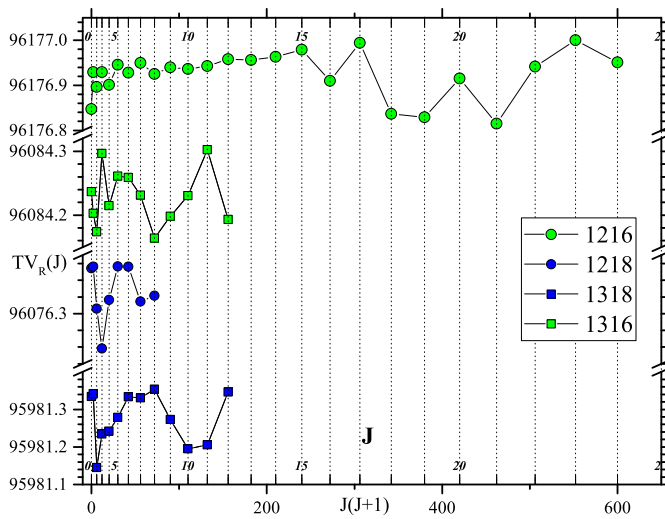


Fig. A.9. Reduced term values (cm^{-1}) of the $C^1\Sigma^+(v'=2)$ levels for the four observed CO isotopologues.

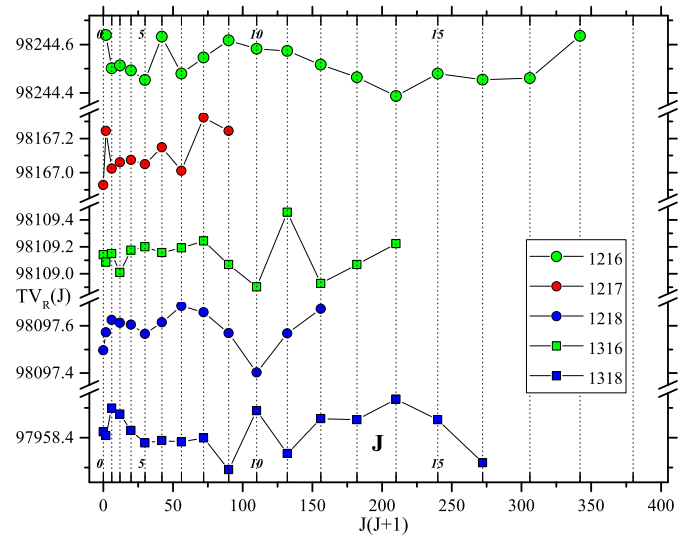


Fig. A.11. Reduced term values (cm^{-1}) of the $C^1\Sigma^+(v'=3)$ levels for the five observed CO isotopologues.

Table A.9. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(\nu' = 0) - X^1\Sigma^+(\nu'' = 0)$ band for $^{12}C^{16}O$, $^{12}C^{17}O$, and $^{12}C^{18}O$ (same column description as for Table A.1).

J''	$^{12}C^{16}O$				$^{12}C^{17}O$				$^{12}C^{18}O$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	$\delta\rho$	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	$\delta\rho$	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	$\delta\rho$
0	108.78678	108.79595	91922.930	-5	108.78708	108.79594	91922.681	-52	108.78724	108.79595	91922.547	-16
1	108.78215	108.80042	91926.842	-10	108.78251	108.80026	91926.542	-58	108.78281	108.80020	91926.288	0
2	108.77744	108.80488	91930.823	23	108.77792	108.80455	91930.420	36	108.77379	108.80448	91930.082	-6
3	108.77274	108.80935	91934.795	-14	108.77334	108.80906	91934.295	-76	108.77022	108.80464	91933.910	-2
4	108.76788	108.81366	91938.903	17	108.76864	108.81307	91938.265	-20	108.76460	108.81279	91937.773	1
5	108.76309	108.81797	91942.952	-15	108.76391	108.81307	91942.265	-13	108.76046	108.81279	91941.681	0
6	108.75815	108.82220	91947.128	17	108.75912	108.81738	91946.310	-2	108.75523	108.81689	91945.629	3
7	108.75329	108.82643	91951.237	-17	108.75432	108.82153	91950.370	3	108.75045	108.82492	91953.642	-11
8	108.74826	108.83058	91955.490	17	108.74945	108.82563	91954.490	2	108.74565	108.82885	91957.701	6
9	108.74324	108.83465	91959.735	-11	108.74455	108.82970	91958.627	-12	108.74080	108.83277	91961.799	-1
10	108.73814	108.83873	91964.048	-4	108.73957	108.83369	91962.839	-11	108.73590	108.83660	91965.944	-1
11	108.73304	108.84272	91968.362	0	108.73458	108.83761	91967.067	-8	108.73096	108.84040	91970.125	2
12	108.72786	108.84663	91972.743	-27	108.72954	108.84149	91971.326	-10	108.72596	108.84415	91974.353	0
13	108.72261	108.85054	91977.184	-19	108.72442	108.84534	91975.661	-12	108.72094	108.84785	91978.605	-8
14	108.71735	108.85438	91981.634	-9	108.71925	108.84914	91980.030	-8	108.71585	108.85146	91982.909	3
15	108.71201	108.85821	91986.153	4	108.71406	108.85285	91984.421	3	108.71071	108.85510	91987.255	-1
16	108.70667	108.86196	91990.671	19	108.70883	108.85653	91988.847	-6	108.70556	108.85863	91991.613	5
17	108.70126	108.86564	91995.250	23	108.70355	108.86019	91993.318	3	108.70035	108.86212	91996.023	-5
18	108.69584	108.86931	91999.837	17	108.69821	108.86376	91997.836	7	108.69508	108.86556	92000.485	-8
19	108.69035	108.87291	92004.484	5	108.69286	108.86731	92002.367	2	108.68978	108.86896	92004.972	-6
20	108.68478	108.87642	92009.199	0	108.68745	108.87079	92006.945	-5	108.68442	108.87228	92009.510	2
21	108.67920	108.87986	92013.923	0	108.68200	108.87422	92011.558	-5	108.67905	108.87558	92014.058	-8
22	108.67363	108.88329	92018.639	-31	108.67650	108.87762	92016.215	-2	108.67360	108.87882	92018.672	9
23	108.66790	108.88665	92023.491	-9	108.67095	108.88094	92020.915	5	108.66812	108.88201	92023.306	6
24	108.66225	108.88976	92028.276	-18	108.66534	108.88422	92025.663	11	108.66262	108.88517	92027.970	0
25	108.65644	108.89328	92033.197	-4	108.65972	108.88744	92030.427	-43	108.65704	108.88825	92032.690	6
26	108.65063	108.89648	92038.118	48	108.65404	108.89061	92035.234	8	108.65145	108.89129	92037.428	-6
27	108.64483	108.89976	92043.032	-18	108.64831	108.89376	92040.089	2	108.64580	108.89427	92042.216	-5
28	108.63894	108.90276	92048.022	37	108.64258	108.89670	92044.945	-81	108.64013	108.89719	92047.018	4
29	108.63289	108.90582	92053.155	62	108.63676	108.89982	92049.875	-44	108.63436	108.90007	92051.910	4
30	108.62687	108.90883	92058.253	43	108.63092	108.90280	92054.823	99	108.63278	108.90291	92056.804	-10
31	108.62088	108.91179	92063.327	66	108.62505	108.90549	92059.796	-22	108.62858	108.90567	92061.720	4
32	108.61481	108.91467	92068.473	47	108.61894	108.90844	92064.974	99	108.62278	108.90839	92066.671	4
33	108.60872	108.91751	92073.638	66	108.61332	108.91132	92069.738	-96	108.61694	108.91107	92071.678	-16
34	108.60260	108.92035	92078.827	51	108.91676				108.61103	108.91367	92076.726	43
35	108.59639	108.92306	92084.091	29					108.60508	108.91621	92081.772	
36	108.59017	108.92572	92089.363						108.59913	108.91885		
37	108.58389		92094.690									
38			91803.503									

Table A.10. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(v'=0)-X^1\Sigma^+(v''=0)$ band for $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$				
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	δp	
0	108.78698	108.79570	91922.763	12	108.78732	108.79581	91922.475	-23	108.78749	108.79581	91922.332	3	
1	108.78251	108.80006	91926.540	11	108.78293	108.79997	91926.184	-28	108.78326	108.79990	91925.906	9	
2	108.77804	108.80429	91930.317	-7	108.77414	108.80405	91933.613	-3	108.77468	108.80395	91933.157	-3	
3	108.77350	108.80848	91934.154	0	108.76968	108.80425	91937.386	26	108.77032	108.80792	91936.842	-5	
4	108.76887	108.81266	91941.973	16	108.76512	108.81232	91941.240	69	108.76587	108.81187	91940.604	-7	
5	108.76425	108.81676	91945.955	6	108.76059	108.81643	91945.073	44	108.76142	108.81577	91944.365	13	
6	108.75954	108.82081	91949.893	9	108.75597	108.82028	91948.978	4	108.75691	108.81963	91948.178	4	
7	108.75488	108.82480	91953.956	6	108.75131	108.82411	91952.917	33	108.75237	108.82342	91952.017	-3	
8	108.75023	108.82873	91958.056	-1	108.74660	108.82802	91956.900	-12	108.74776	108.82715	91955.915	-2	
9	108.74553	108.83269	91962.130	0	108.74185	108.83171	91960.911	-10	108.74316	108.83087	91959.804	10	
10	108.74041	108.83653	91966.319	-14	108.73707	108.83547	91964.959	-29	108.73846	108.83454	91963.779	-11	
11	108.73546	108.84036	91970.491	1	108.73224	108.83913	91969.045	-12	108.73372	108.83814	91967.788	-5	
12	108.73053	108.84412	91974.733	-7	108.72732	108.84283	91973.203	3	108.72894	108.84170	91971.831	-6	
13	108.72551	108.84784	91979.057	1	108.72242	108.84648	91977.349	3	108.72411	108.84520	91975.918	-1	
14	108.72050	108.85146	91983.354	24	108.71740	108.85000	91981.595	-5	108.71925	108.84867	91980.029	-6	
15	108.71532	108.85512	91987.688	3	108.71240	108.85352	91985.830	1	108.71433	108.85206	91984.191	-2	
16	108.71020	108.85865	91992.080	-11	108.70734	108.85694	91990.109	3	108.70939	108.85544	91988.371	1	
17	108.70501	108.86215	91996.504	-6	108.70223	108.86037	91994.430	-2	108.70438	108.85875	91992.616	-7	
18	108.69978	108.86562	92000.988	-5	108.69709	108.86372	91998.782	-6	108.69936	108.86201	91996.865	7	
19	108.69448	108.86903	92005.489	-1	108.69188	108.86702	92003.193	-5	108.69426	108.86524	92001.176	-4	
20	108.68917	108.87238	92010.033	-11	108.68663	108.87028	92007.634	10	108.68914	108.86840	92005.510	6	
21	108.68380	108.87566	92014.628	-8	108.68135	108.87351	92012.105	7	108.68395	108.87153	92009.903	-4	
22	108.67837	108.87892	92019.251	7	108.67604	108.87665	92016.604	1	108.67876	108.87458	92014.297	0	
23	108.67291	108.88214	92023.871	13	108.67065	108.87974	92021.164	-6	108.67347	108.87759	92018.776	-6	
24	108.66746	108.88530	92028.583	3	108.66525	108.88279	92025.736	2	108.66817	108.88056	92023.267	-4	
25	108.66189	108.88842	92033.286	3	108.65980	108.88579	92030.358	-8	108.66284	108.88345	92027.778	0	
26	108.65634	108.89148	92038.051	8	108.65426	108.88873	92035.049	-28	108.65746	108.88632	92032.340	0	
27	108.65071	108.89447	92042.851	5	108.64877	108.89158	92039.699	11	108.65203	108.88915	92036.935	-5	
28	108.64505	108.89741	92047.685	2	108.64318	108.89448	92044.437	-9	108.64657	108.89190	92041.558	-12	
29	108.63934	108.90030	92052.558	3	108.63753	108.89728	92049.219	-2	108.64108	108.89460	92046.214	4	
30	108.63359	108.90314	92057.459	4	108.63177	108.90003	92054.105	1	108.63552	108.89731	92050.924	1	
31	108.62781	108.90593	92062.416	-3	108.62609	108.90271	92058.917	39	108.62992	108.89993	92055.671	-4	
32	108.62196	108.90866	92067.399	8	108.62039	108.90534	92063.747	27	108.62429	108.90247	92060.442	-4	
33	108.61608	108.91135	92072.405	11	108.61468	108.90793	92068.583	29	108.61863	108.90496	92065.241	7	
34	108.61017	108.91399	92077.453	13	108.60882	108.91075	92073.551	3	108.61291	108.90745	92070.086	-4	
35	108.60422	108.91658	92082.526	-16	108.60289	108.91309	92078.579	29	108.60715	108.90984	92074.967	2	
36	108.59824	108.91901	92087.637	-29	108.59743	108.91542	92083.214	-1	108.60135	108.91221	92079.883	8	
37	108.59221	108.92152	92092.778	1	108.59170	108.91775	92088.071	3	108.59553	108.91453	92084.825	2	
38	108.58615	108.92439	92098.076	1	108.58576	108.91898	92093.830	8	108.58971	108.91676	92089.754	8	
39	108.57990				108.57783	108.92111	92099.830	-27	108.58376	108.91898	92094.807	8	
40					108.57598	108.92439	92109.574	*	108.57798	108.92111	92099.830	*	
41													
42													
43													

Table A.11. Term values (cm^{-1}) of the $C^1\Sigma^+(v'=0)$ levels for six CO isotopologues.

J'	$C^1\Sigma^+(v'=0)$					
	$^{12}C^{16}O$	$^{12}C^{17}O$	$^{12}C^{18}O$	$^{13}C^{16}O$	$^{13}C^{17}O$	$^{13}C^{18}O$
0	91919.027	91918.939	91918.851	91919.074	91918.886	91918.794
1	91922.935 (-5)	91922.733 (-52)	91922.563 (-16)	91922.751 (12)	91922.499 (-23)	91922.329 (3)
2	91930.698 (-10)	91930.348 (-58)	91929.950 (0)	91930.204 (11)	91929.791 (-28)	91929.390 (9)
3	91942.334 (23)	91941.627 (36)	91941.074 (-6)	91941.352 (-7)	91940.580 (-3)	91939.995 (-3)
4	91957.879 (-14)	91956.858 (-76)	91955.883 (-2)	91956.209 (0)	91955.059 (26)	91954.118 (-5)
5	91977.334 (17)	91975.760 (-20)	91974.389 (1)	91974.809 (16)	91973.103 (69)	91971.775 (-7)
6	92000.638 (-15)	91998.492 (-13)	91996.606 (0)	91997.101 (6)	91994.873 (44)	91992.978 (13)
7	92027.846 (17)	92025.008 (-2)	92022.518 (3)	92023.131 (9)	92020.214 (4)	92017.701 (4)
8	92058.896 (-17)	92055.291 (3)	92052.127 (-11)	92052.837 (-35)	92049.134 (33)	92045.965 (-3)
9	92093.891 (-11)	92089.383 (2)	92085.437 (6)	92086.262 (-1)	92081.738 (-12)	92077.734 (-2)
10	92132.717 (-4)	92127.249 (-12)	92122.444 (-1)	92123.428 (0)	92117.912 (-10)	92113.041 (10)
11	92175.452 (0)	92168.915 (-11)	92163.141 (-1)	92164.253 (-14)	92157.710 (-29)	92151.859 (-11)
12	92222.056 (-27)	92214.337 (-8)	92207.535 (2)	92208.833 (1)	92201.079 (-12)	92194.222 (-5)
13	92272.528 (-19)	92263.533 (-10)	92255.623 (0)	92257.085 (-7)	92248.060 (3)	92240.111 (-6)
14	92326.890 (-9)	92316.541 (-12)	92307.416 (-8)	92309.080 (-22)	92298.695 (3)	92289.512 (-1)
15	92385.092 (4)	92373.313 (-8)	92362.863 (3)	92364.760 (24)	92352.893 (-5)	92342.447 (-6)
16	92447.188 (19)	92433.835 (3)	92422.025 (-1)	92424.142 (3)	92410.744 (1)	92398.878 (-2)
17	92513.139 (7)	92498.140 (-6)	92484.867 (5)	92487.214 (-11)	92472.151 (3)	92458.840 (1)
18	92582.947 (23)	92566.203 (3)	92551.379 (-5)	92553.982 (-6)	92537.171 (-2)	92522.307 (-7)
19	92656.609 (17)	92638.044 (7)	92621.572 (-3)	92624.441 (-5)	92605.790 (-6)	92589.290 (7)
20	92734.156 (5)	92713.634 (-1)	92695.465 (-8)	92698.610 (-1)	92677.993 (-5)	92659.775 (-4)
21	92815.581 (1)	92792.982 (2)	92773.012 (-6)	92776.462 (-11)	92753.795 (10)	92733.771 (6)
22	92900.825 (0)	92876.094 (-5)	92854.237 (2)	92857.991 (-8)	92833.197 (7)	92811.277 (-4)
23	92989.903 (-31)	92962.954 (-2)	92939.122 (-8)	92943.203 (7)	92916.182 (1)	92892.294 (0)
24	93082.854 (9)	93053.576 (-4)	93027.674 (9)	93032.096 (13)	93002.743 (-6)	92976.784 (-6)
25	93179.610 (-18)	93147.943 (5)	93119.891 (6)	93124.638 (3)	93092.894 (2)	93064.809 (-4)
26	93280.260 (-4)	93246.036 (11)	93215.764 (0)	93220.881 (22)	93186.615 (-8)	93156.301 (0)
27	93384.671 (48)	93347.935 (-43)	93315.298 (6)	93320.780 (8)	93283.933 (-28)	93251.270 (0)
28	93492.986 (-18)	93453.476 (8)	93418.485 (-6)	93424.358 (5)	93384.795 (11)	93349.746 (-5)
29	93605.101 (-18)	93562.769 (2)	93525.320 (-5)	93531.596 (2)	93489.206 (-9)	93451.704 (-12)
30	93721.089 (37)	93675.906 (-81)	93635.779 (-5)	93642.487 (3)	93597.205 (-2)	93557.111 (4)
31	93840.854 (62)	93792.627 (-44)	93749.921 (4)	93757.034 (4)	93708.777 (1)	93666.009 (1)
32	93964.415 (43)	93913.072 (-22)	93867.675 (4)	93875.231 (-3)	93823.936 (39)	93778.401 (-4)
33	94091.798 (47)	94037.302 (99)	93989.048 (4)	93997.075 (8)	93942.588 (27)	93894.258 (-4)
34	94222.951 (66)	94165.107 (-96)	94114.061 (-10)	94122.558 (11)	94064.784	94013.556 (7)
35	94357.931 (47)		94242.709 (-16)	94251.666 (13)	94190.438 (29)	94136.329 (-4)
36	94496.720 (51)		94374.916 (43)	94384.456 (-29)	94319.787 (-1)	94262.552 (2)
37	94639.295 (29)		94510.802	94520.809 (-16)	94452.659 (3)	94392.228 (8)
38	94785.681			94660.782	94588.641	94525.363 (2)
39				94804.384	94728.331	94661.919 (8)
40				94951.719		94801.907 (-27)
41						94944.865 (*)
42						95092.196
43						95237.275
44						95395.735

Notes. The δ_p value in parentheses (in units of the least significant digit) corresponds to the wavenumber correction applied to TV_P and TV_R . There is no value when the term value is derived from a single transition, either R or P . An asterisk indicates when both R - and P -branches are present at high J' , either the potential presence of a perturbing state or that one of the lines shows a larger uncertainty than the other (see also Sect. 2.2.2).

Table A.12. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(v' = 1) - X^1\Sigma^+(v'' = 0)$ band for $^{12}C^{16}O$, $^{12}C^{17}O$, and $^{12}C^{18}O$ (same column description as for Table A.1).

J''	$^{12}C^{16}O$					$^{12}C^{17}O$					$^{12}C^{18}O$				
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δP	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	P_{ms} (cm $^{-1}$)	δP
0	106.30450	106.31320	94069.392	94061.694	-7	106.33521	106.34360	94042.231	94034.805	-22	106.36264	106.37095	94017.971	94010.626	0
1	106.30013	106.31752	94073.259	94057.872	-12	106.33096	106.34787	94045.990	94031.033	-7	106.35852	106.37507	94021.613	94006.985	-25
2	106.29575	106.32183	94077.135	94054.059	23	106.32670	106.35213	94049.756	94027.265	15	106.35433	106.37918	94025.318	94003.353	-14
3	106.29143	106.32622	94080.959	94050.175	-3	106.32243	106.35640	94053.531	94023.493	22	106.35012	106.38330	94029.031	93999.713	-2
4	106.28705	106.33053	94084.836	94046.363	3	106.31817	106.36062	94057.300	94019.761	10	106.34602	106.38742	94032.665	93996.073	-21
5	106.28268	106.33485	94088.704	94042.542	5	106.31391	106.36480	94061.066	94016.061	2	106.34182	106.39154	94036.379	93992.433	-4
6	106.27830	106.33917	94092.582	94038.722	13	106.30965	106.36900	94064.835	94012.353	-2	106.33763	106.39566	94040.084	93988.793	10
7	106.27399	106.34349	94096.398	94034.902	-10	106.30540	106.37320	94068.602	94008.641	-3	106.33344	106.39978	94043.790	93985.153	25
8	106.26961	106.34781	94100.276	94031.082	0	106.30113	106.37741	94072.379	94004.922	2	106.32933	106.40390	94047.425	93981.514	-26
9	106.26523	106.35213	94104.155	94027.263	11	106.29685	106.38162	94076.165	94001.204	1	106.32513	106.40795	94051.140	93977.937	-4
10	106.26086	106.35645	94108.025	94023.443	19	106.29259	106.38580	94079.935	93997.511	-3	106.32094	106.41207	94058.553	93974.299	14
11	106.25654	106.36077	94111.851	94019.624	7	106.28833	106.38998	94083.704	93993.810	-6	106.31675	106.42428	94065.967	93970.660	-1
12	106.25217	106.36509	94115.722	94015.806	-7	106.28404	106.39417	94087.499	93990.109	-5	106.31256	106.42833	94069.666	93963.517	-18
13	106.24779	106.36935	94119.601	94012.041	11	106.27976	106.39834	94091.294	93986.430	14	106.30837	106.43245	94073.374	93959.941	3
14	106.24342	106.37367	94123.473	94008.223	-4	106.27548	106.40254	94095.082	93982.719	14	106.30419	106.43649	94077.153	93956.304	-4
15	106.23905	106.37792	94127.344	94004.467	19	106.27122	106.40670	94098.852	93979.043	-1	106.30000	106.44054	94080.861	93952.738	30
16	106.23467	106.38225	94131.225	94000.641	17	106.26695	106.41085	94102.639	93975.381	-2	106.29573	106.44451	94084.561	93949.163	-4
17	106.23036	106.38651	94135.044	93996.877	-17	106.26267	106.41500	94106.428	93971.716	-7	106.29154	106.44856	94088.271	93945.659	-5
18	106.22599	106.39076	94138.917	93993.122	13	106.25840	106.41913	94110.206	93968.063	11	106.28736	106.45261	94091.980	93942.085	1
19	106.22162	106.39509	94142.790	93989.296	16	106.25410	106.42333	94114.012	93964.360	4	106.28317	106.45666	94095.690	93938.511	10
20	106.21724	106.39935	94146.672	93985.533	-5	106.24984	106.42743	94117.785	93960.741	-13	106.27898	106.46063	94099.462	93934.937	-13
21	106.21294	106.40354	94150.483	93981.832	-28	106.24554	106.43154	94121.600	93957.114	-23	106.27479	106.46460	94103.163	93931.434	-3
22	106.20856	106.40780	94154.366	93978.070	-7	106.24127	106.43561	94125.379	93953.519	*	106.27053	106.46857	94106.873	93927.931	-24
23	106.20419	106.41207	94158.240	93974.299	8	106.23699	106.44012	94129.175	93949.534	*	106.26635	106.47254	94110.584	93924.429	-42
24	106.19989	106.41633	94162.053	93970.537	-4	106.23275	106.44419	94132.927	93945.943	*	106.26216	106.47643	94114.294	93920.933	-87
25	106.19551	106.42059	94165.936	93966.775	6	106.22878	106.44832	94137.251	93942.297	*	106.25797	106.48060	94118.122	93917.500	-4
26	106.19121	106.42481	94169.750	93963.048	5	106.22494	106.45237	94141.623	93938.724	*	106.25379	106.48385	94121.778	93913.817	*
27	106.18684	106.42908	94173.625	93959.280	-8	106.22127	106.45652	94146.158	93935.192	*	106.24946	106.48713	94125.599	93910.957	*
28	106.18251	106.43324	94177.471	93955.606	-6	106.21782	106.46067	94150.192			106.24534	106.49060	94129.342	93908.060	
29	106.17821	106.43746	94181.283	93951.883	-6	106.21327					106.24102	106.49460	94132.877		
30	106.17386	106.44171	94185.143	93948.135	9						106.23680				
31	106.16958	106.44592	94189.935	93944.416	-33						106.23261				
32	106.16526														
33															

Table A.13. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(\nu' = 1) - X^1\Sigma^+(\nu'' = 0)$ band for $^{13}\text{C}^{16}\text{O}$, $^{13}\text{C}^{17}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	P_{ms} (cm^{-1})	δP	R_{ms} (nm)	P_{ms} (nm)	P_{ms} (cm^{-1})	δP	R_{ms} (nm)	P_{ms} (nm)	P_{ms} (cm^{-1})	δP
0	106.35798	106.36630	94022.091	-38	106.38925	106.39786	93994.456	79	106.41767	106.42556	93969.353	-17
1	106.35378	106.37037	94025.804	-63	106.38582	106.40159	93997.486	-93	106.41366	106.42950	93972.895	0
2	106.34953	106.37443	94029.561	*	106.38175	106.40587	94001.082	-18	106.40972	106.43344	93976.374	-9
3	106.34565	106.37888	94032.992	-81	106.37762	106.41077	94004.732	-16	106.40571	106.43739	93979.916	9
4	106.34108	106.38289	94037.033	59	106.37371	106.41404	94008.187	*	106.40177	106.44133	93983.396	-25
5	106.33689	106.38695	94040.738	9	106.36942	106.41802	94011.979	-36	106.39776	106.44522	93986.938	-6
6	106.33276	106.39096	94044.391	-13	106.36529	106.42199	94015.629	-19	106.39369	106.44916	93990.533	13
7	106.32857	106.39509	94048.097	-7	106.36123	106.42600	94019.222	-27	106.38969	106.45304	93994.067	8
8	106.32444	106.40036	94051.750	-23	106.35716	106.43001	94022.816	-20	106.38575	106.45693	93997.548	-1
9	106.32019	106.40536	94055.510	-15	106.35309	106.43400	94026.414	-53	106.38174	106.46087	94001.091	-31
10	106.31593	106.41036	94059.278	-1	106.34894	106.43799	94030.744	-33	106.37768	106.46469	94004.679	-12
11	106.31206	106.41589	94062.702	-17	106.34480	106.44197	94033.744	53	106.37367	106.46857	94011.758	-8
12	106.30756	106.42150	94066.684	*	106.34087	106.44611	94037.223	-22	106.36967	106.47246	94015.355	-12
13	106.30337	106.42743	94070.392	63	106.33658	106.45008	94041.013	32	106.36560	106.47634	94018.944	-9
14	106.29943	106.43396	94073.878	-58	106.33246	106.45399	94044.661	48	106.36154	106.48016	94022.542	21
15	106.29512	106.44019	94077.693	-8	106.32846	106.45797	94048.203	16	106.35747	106.48405	94026.078	4
16	106.29080	106.44643	94081.516	36	106.32430	106.46189	94051.878	56	106.35347	106.48781	94029.623	-4
17	106.28655	106.45211	94085.278	-34	106.32013	106.46587	94055.563	27	106.34946	106.49169	94033.213	-12
18	106.28236	106.45824	94089.988	39	106.31598	106.46978	94059.239	49	106.34540	106.49551	94036.812	-16
19	106.27824	106.46409	94092.635	10	106.31185	106.47373	94062.893	50	106.34133	106.49933	94040.455	24
20	106.27399	106.47026	94096.398	-5	106.30773	106.47764	94066.538	67	106.33721	106.50309	94044.108	44
21	106.26980	106.47634	94100.108	14	106.30354	106.48156	94070.246	34	106.33308	106.50691	94047.593	-17
22	106.26555	106.48234	94103.871	5	106.29947	106.48544	94073.843	56	106.32914	106.51067	94051.184	-23
23	106.26137	106.48836	94107.573	14	106.29532	106.48932	94077.520	*	106.32508	106.51443	94054.793	15
24	106.25718	106.49436	94111.284	36	106.29118	106.49324	94081.477	*	106.32100	106.51819	94058.387	-14
25	106.25293	106.50036	94115.048	29	106.28706	106.49720	94085.185	*	106.31694	106.52202	94062.002	1
26	106.24875	106.50636	94118.751	-35	106.28294	106.50102	94088.921	*	106.31286	106.52571	94065.581	-25
27	106.24450	106.51236	94122.516	34	106.27882	106.50484	94092.626	*	106.30881	106.52947	94069.195	-8
28	106.24032	106.51836	94126.219	*	106.27470	106.50866	94096.393	*	106.30473	106.53317	94072.791	24
29	106.23611	106.52436	94129.953	*	106.27058	106.51242	94100.095	*	106.30066	106.53692	94076.367	44
30	106.23191	106.53036	94133.678	*	106.26646	106.51616	94103.832	*	106.29662	106.54069	94080.021	24
31	106.22771	106.53636	94137.398	*	106.26234	106.51995	94107.520	*	106.29249	106.54443	94083.735	44
32	106.22353	106.54236	94141.189	*	106.25822	106.52371	94111.032	*	106.28836	106.54817	94087.475	24
33	106.21927	106.54836	94144.877	*	106.25410	106.52743	94114.823	*	106.28424	106.55191	94091.219	44
34	106.21510	106.55436	94148.571	*	106.25006	106.53116	94118.641	*	106.28012	106.55565	94095.062	24
35	106.21083	106.56036	94152.357	*	106.24594	106.53490	94122.433	*	106.27600	106.55939	94098.807	44
36	106.20666	106.56636	94156.051	*	106.24182	106.53852	94126.225	*	106.27188	106.56313	94102.551	24
37		106.57236		*	106.23770		94130.067	*				
38		106.57836		*	106.23358		94133.862	*				
39		106.58436		*	106.22946		94137.657	*				
40		106.59036		*	106.22534		94141.451	*				
41		106.59636		*	106.22122		94145.246	*				
42		106.60236		*	106.21710		94149.041	*				
43		106.60836		*	106.21308		94152.836	*				
44		106.61436		*	106.20906		94156.631	*				
45		106.62036		*	106.20504		94160.426	*				

Table A.14. Term values (cm⁻¹) of the C¹Σ⁺(v' = 1) levels for six CO isotopologues.

J'	C ¹ Σ ⁺ (v' = 1)					
	¹² C ¹⁶ O	¹² C ¹⁷ O	¹² C ¹⁸ O	¹³ C ¹⁶ O	¹³ C ¹⁷ O	¹³ C ¹⁸ O
0	94065.539	94038.553	94014.288	94018.412	93990.428	93965.880
1	94069.399 (-7)	94042.254 (-22)	94017.971 (0)	94022.129 (-38)	93994.252 (*)	93969.370 (-17)
2	94077.116 (-12)	94049.745 (-7)	94025.300 (-25)	94029.543 (-63)	94001.158 (-93)	93976.387 (0)
3	94088.647 (23)	94060.985 (15)	94036.317 (-14)	94040.482 (107)	94011.837 (-18)	93986.861 (-9)
4	94104.031 (-3)	94075.996 (22)	94050.999 (2)	94055.128 (-81)	94026.220 (-16)	94000.863 (9)
5	94123.281 (3)	94094.767 (10)	94069.303 (-21)	94073.731 (59)	94044.084 (*)	94018.347 (-25)
6	94146.370 (5)	94117.278 (2)	94091.307 (-4)	94095.863 (9)	94065.692 (-36)	94039.332 (-6)
7	94173.305 (13)	94143.533 (-2)	94116.965 (10)	94121.589 (-13)	94090.793 (-19)	94063.860 (13)
8	94204.050 (-10)	94173.529 (-3)	94146.282 (25)	94151.013 (-7)	94119.439 (-27)	94091.842 (8)
9	94238.667 (0)	94207.272 (2)	94179.252 (-26)	94184.078 (-23)	94151.645 (-20)	94123.265 (-1)
10	94277.122 (11)	94244.774 (1)	94215.887 (-4)	94220.897 (-15)	94187.469 (-53)	94158.259 (-31)
11	94319.409 (19)	94286.003 (-3)	94256.173 (14)	94261.389 (-1)	94226.890 (-33)	94196.734 (-12)
12	94365.511 (7)	94330.972 (-6)	94300.147 (-1)	94305.234 (-17)	94269.799 (53)	94238.669 (-8)
13	94415.494 (-7)	94379.701 (-5)	94347.768 (-10)	94353.165 (106)	94316.262 (-22)	94284.086 (-12)
14	94469.288 (11)	94432.149 (14)	94399.040 (-18)	94404.654 (63)	94366.475 (32)	94333.044 (-9)
15	94526.938 (-4)	94488.344 (14)	94453.924 (3)	94459.663 (-58)	94420.153 (48)	94385.446 (21)
16	94588.380 (19)	94548.269 (-1)	94512.494 (-4)	94518.492 (-8)	94477.368 (-14)	94441.388 (1)
17	94653.683 (17)	94611.929 (-2)	94574.739 (30)	94580.988 (44)	94538.186 (16)	94500.723 (4)
18	94722.782 (-17)	94679.323 (-7)	94640.626 (-4)	94647.134 (40)	94602.595 (27)	94563.564 (-12)
19	94795.693 (13)	94750.410 (11)	94710.113 (-5)	94716.881 (39)	94670.543 (49)	94629.898 (-4)
20	94872.451 (16)	94825.275 (4)	94783.241 (1)	94790.247 (10)	94742.049 (50)	94699.734 (-16)
21	94953.060 (-5)	94903.838 (-13)	94860.003 (10)	94867.346 (14)	94817.102 (48)	94773.033 (24)
22	95037.414 (-28)	94986.153 (-23)	94940.432 (-13)	94948.063 (-5)	94895.749 (67)	94849.828 (44)
23	95125.607 (-7)	95071.968 (*)	95024.520 (-3)	95032.448 (5)	94977.888 (34)	94930.001 (-17)
24	95217.604 (8)	95161.698 (*)	95112.198 (-24)	95120.416 (14)	95063.597 (56)	95013.686 (-23)
25	95313.372 (-4)	95255.084 (*)	95203.506 (-42)	95212.019 (36)	95152.969 (*)	95100.807 (15)
26	95412.990 (6)	95352.495 (*)	95298.465 (-87)	95307.339 (29)	95245.814 (*)	95191.435 (-14)
27	95516.346 (5)	95454.281	95396.912 (-4)	95406.288 (-35)	95342.207 (*)	95285.493 (1)
28	95623.569 (-8)	95559.553	95499.443 (*)	95508.862 (-34)	95442.113 (*)	95383.007 (-25)
29	95734.539 (-6)	95668.018	95605.477 (*)	95615.111 (*)	95545.608 (*)	95483.960 (-8)
30	95849.260 (-6)		95714.354	95724.997 (*)	95652.600 (*)	95588.347
31	95967.797 (9)		95827.358	95838.431 (*)	95763.109 (*)	95696.164
32	96090.099 (-33)		95943.752	95955.503 (*)	95877.478 (*)	95807.494
33	96216.142			96076.216 (*)	95995.073 (*)	95921.819
34				96200.504 (*)	96116.172 (*)	
35				96328.391 (*)	96240.783 (*)	
36				96459.893 (*)	96368.929 (*)	
37				96594.952 (*)	96501.308	
38				96734.237	96636.494	
39				96876.548	96775.059	
40				97022.430	96917.129	
41				97171.950	97062.777	
42				97324.945	97211.828	
43				97481.067		
44				97641.214		

Notes. See note to Table A.11.

Table A.15. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(v'=2)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{12}\text{C}^{16}\text{O}$					$^{12}\text{C}^{18}\text{O}$				
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	P_{ms} (cm^{-1})	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	P_{ms} (cm^{-1})	δ_P
0	103.97097	103.97929	96180.696	96173.002	-39	104.07997	104.08785	96079.966	96072.692	-10
1	103.96690	103.98335	96184.460	96169.239	-8	104.07616	104.09185	96083.483	96069.001	-21
2	103.96283	103.98767	96188.222	96165.252	-5	104.07236	104.09595	96086.992	96065.217	-4
3	103.95889	103.99192	96191.872	96161.320	-14	104.06851	104.10012	96090.547	96061.369	-10
4	103.95488	103.99627	96195.579	96157.299	2	104.06469	104.10419	96094.074	96057.613	8
5	103.95100	104.00060	96199.174	96153.289	7	104.06103	104.10834	96097.454	96053.784	-52
6	103.94711	104.00504	96202.769	96149.188	13	104.05726	104.11248	96100.935	96049.964	55
7	103.94335	104.00947	96206.251	96145.089	-9	104.05355	104.11687	96104.362	96045.915	75
8	103.93953	104.01397	96209.789	96140.933	27	104.05000	104.12113	96107.800	96041.985	55
9	103.93583	104.01853	96213.215	96136.721	9	104.04649	104.12620	96111.237	96037.309	75
10	103.93213	104.02308	96216.641	96132.508	20					
11	103.92849	104.02770	96220.010	96128.240	4					
12	103.92491	104.03232	96223.324	96123.971	-9					
13	103.92133	104.03700	96226.638	96119.647	7					
14	103.91781	104.04175	96229.896	96115.266	-2					
15	103.91441	104.04649	96233.040	96110.886	*					
16	103.91090	104.05124	96236.298	96107.066						
17	103.90768	104.05602	96239.275							
18	103.90435		96242.364							
19	103.90095		96245.509							
20	103.89780		96248.430							
21	103.89444		96251.540							

J''	$^{13}\text{C}^{16}\text{O}$					$^{13}\text{C}^{18}\text{O}$				
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	P_{ms} (cm^{-1})	δ_P	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm^{-1})	P_{ms} (cm^{-1})	δ_P
0	104.07148	104.07933	96087.808	96080.561	-35	104.18328	104.19072	95984.695	95977.841	-99
1	104.06751	104.08335	96091.474	96076.850	56	104.17968	104.19444	95988.012	95974.415	1
2	104.06364	104.08754	96095.047	96072.982	-60	104.17596	104.19864	95991.440	95970.546	-36
3	104.05977	104.09138	96098.621	96069.438	64	104.17231	104.20242	95994.803	95967.065	-23
4	104.05604	104.09574	96102.066	96065.414	-33	104.16865	104.20638	95998.176	95963.418	0
5	104.05227	104.09976	96105.548	96061.705	-10	104.16506	104.21035	96001.484	95959.762	-36
6	104.04856	104.10400	96108.974	96057.792	19	104.16146	104.21426	96004.802	95956.162	11
7	104.04497	104.10831	96112.291	96053.815	13	104.15793	104.21834	96008.056	95952.405	-23
8	104.04133	104.11266	96115.653	96049.802	-16	104.15445	104.22231	96011.264	95948.750	75
9	104.03768	104.11691	96119.025	96045.881		104.15098	104.22620	96014.463	96017.772	75
10	104.03404		96122.388			104.14739		96017.772		
11	104.03063		96125.539			104.14362		96021.248		

Table A.16. Term values (cm^{-1}) of the $C^1\Sigma^+(v'=2)$ levels for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$.

J'	$C^1\Sigma^+(v'=2)$					
	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	96176.847		96076.354	96084.237		95981.334
1	96180.735 (–39)		96079.976 (–10)	96087.843 (–35)		95984.794 (–99)
2	96188.313 (–8)		96087.167 (–21)	96095.093 (56)		95991.504 (1)
3	96199.763 (–5)		96097.982 (–4)	96106.135 (–60)		96001.954 (–36)
4	96214.956 (–14)		96112.527 (–10)	96120.612 (64)		96015.782 (–23)
5	96234.026 (2)		96130.683 (8)	96138.856 (–33)		96033.102 (0)
6	96256.838 (7)		96152.430 (–52)	96160.691 (–10)		96053.908 (–36)
7	96283.492 (13)		96177.772 (55)	96186.140 (19)		96078.132 (11)
8	96313.902 (–9)		96206.804 (75)	96215.187 (13)		96105.863 (–23)
9	96348.152 (27)		96238.649	96247.974 (–16)		96136.979
10	96386.184 (9)			96284.397		96171.599
11	96428.026 (20)			96324.497		96209.816
12	96473.673 (4)			96368.054		96251.686
13	96523.099 (–9)					
14	96576.328 (7)					
15	96633.359 (–2)					
16	96694.441 (*)					
17	96758.774					
18	96826.996					
19	96899.153					
20	96975.186					
21	97054.812					
22	97138.442					

Notes. See note to Table A.11.

Table A.17. Transition wavelengths and wavenumbers of the $C^1\Sigma^+(\nu''=3)-X^1\Sigma^+(\nu''=0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ (same column description as for Table A.1).

J''	$^{12}\text{C}^{16}\text{O}$				$^{12}\text{C}^{17}\text{O}$				$^{12}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp
0	101.78276	98248.469	98240.438	78	101.86301	98171.062	98174.175	*	101.93560	98101.159	98104.744	8
1	101.77912	98251.976	98236.778	65	101.85978	101.87119	98174.175	*	101.93187	98104.744	98093.834	8
2	101.77549	98255.483	98232.621	-4	101.85626	101.87502	98177.568	-61	101.92835	98108.129	98090.158	44
3	101.77189	98258.962	98228.577	26	101.85256	101.87910	98181.135	*	101.92494	98111.413	98086.346	27
4	101.76846	98262.276	98224.309	2	101.84916	101.88313	98184.412	10	101.92154	98114.689	98082.443	-13
5	101.76485	98265.758	98220.309	2	101.84564	101.88758	98187.806	31	101.91818	98117.920	98078.486	48
6	101.76171	98268.790	98219.985	20	101.84237	101.89200	98190.958	*	101.91499	98120.995	98074.319	55
7	101.75845	98271.935	98215.746	12	101.83925	101.89647	98193.966	*	101.91191	98123.961	98070.216	-38
8	101.75520	98275.081	98211.110	-9	101.83629	101.90136	98196.821	*	101.90893	98126.827	98066.160	-70
9	101.75223	98277.945	98206.618	56	101.83308	98201.956	98199.916		101.90591	98129.738	98061.876	-71
10	101.74933	98280.744	98202.956	37	101.83026	98202.635	98202.635		101.90293	98132.605	98057.429	*
11	101.74660	98283.385	98197.182	15	101.82568	98207.053	98207.053		101.89995	98135.471	98052.647	
12	101.74380	98286.089	98192.352	-27								
13	101.74135	98288.459	98187.409	76								
14	101.73857	98291.144	98182.242	-43								
15	101.73601	98293.615	98177.188	67								
16	101.73368	98295.861	98171.996	*								
17	101.73165	98297.827	98166.618	91								
18	101.72977	98299.643	98161.366	*								
19	101.72763	98301.712	98156.578	14								
20	101.88485		98150.022	34								
21	101.89066		98144.419									
22	101.89751		98137.827									

J''	$^{13}\text{C}^{16}\text{O}$				$^{13}\text{C}^{17}\text{O}$				$^{13}\text{C}^{18}\text{O}$			
	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp	R_{ms} (nm)	P_{ms} (nm)	R_{ms} (cm $^{-1}$)	δp
0	101.92352	98112.780	98105.474	93	102.08055	97961.854	97965.280	14	102.07698	97965.280	97954.935	14
1	101.91994	98116.226	98101.567	-31	102.07360	97968.524	97971.720	-5	102.07360	97968.524	97951.347	-5
2	101.91646	98119.577	98097.910	33	102.07027	97971.720	97974.826	-23	102.06700	97974.826	97947.826	-23
3	101.91288	98123.023	98093.782	-28	102.06390	97977.834	97980.858	16	102.06075	97977.834	97944.123	16
4	101.90949	98126.287	98090.000	-50	102.05766	97983.825	97986.571	-7	102.05480	97983.825	97940.257	56
5	101.90619	98129.465	98085.959	-8	102.05176	97989.490	97992.063	-43	102.04908	97989.490	97936.334	-43
6	101.90284	98132.691	98081.707	82	102.04621	97992.063	97994.819	30	102.04347	97992.063	97928.498	30
7	101.89989	98135.532	98077.407	*	102.04105	97997.775	97999.451	44	102.03883	97997.775	97924.413	44
8	101.89694	98138.373	98073.367	-81	102.03883	98001.907	98001.907	6	102.03462	98001.907	97920.155	6
9	101.89399	98141.214	98068.731	55	102.03462	98001.907	98001.907	46	102.03063	98001.907	97916.176	46
10	101.89086	98144.229	98063.961	*	102.03063	98001.907	98001.907	92	102.02635	98001.907	97911.699	92
11	101.88828	98146.714	98060.317		102.02635	98001.907	98001.907	*	102.02212	98001.907	97907.395	*
12	101.88537	98149.517			102.02212	98001.907	98001.907	58	102.01812	98001.907	97902.803	58
13	101.88251	98152.273			102.01812	98001.907	98001.907	-65	102.01462	98001.907	97898.490	-65
14					102.01462	98001.907	98001.907		102.01140	98001.907	97893.909	
15					102.01140	98001.907	98001.907		102.00883	98001.907	97888.974	
16					102.00883	98001.907	98001.907					
17												

Table A.18. Term values (cm^{-1}) of the $C^1\Sigma^+(v' = 3)$ levels for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$, $^{13}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{18}\text{O}$.

J'	$C^1\Sigma^+(v' = 3)$					
	$^{12}\text{C}^{16}\text{O}$	$^{12}\text{C}^{17}\text{O}$	$^{12}\text{C}^{18}\text{O}$	$^{13}\text{C}^{16}\text{O}$	$^{13}\text{C}^{17}\text{O}$	$^{13}\text{C}^{18}\text{O}$
0	98244.283	98166.927	98097.496	98109.150		97958.428
1	98248.391 (78)	98170.897 (*)	98101.151 (8)	98112.687 (93)		97961.839 (14)
2	98255.756 (65)	98177.984 (−61)	98108.361 (44)	98119.934 (−31)		97968.777 (−5)
3	98267.022 (−4)	98188.982 (*)	98119.088 (27)	98130.572 (33)		97979.025 (−23)
4	98282.005 (26)	98203.612 (10)	98133.397 (−13)	98145.106 (−28)		97992.660 (16)
5	98300.722 (2)	98221.858 (31)	98151.258 (48)	98163.094 (−50)		98009.729 (56)
6	98323.408 (20)	98243.884 (*)	98172.789 (55)	98184.608 (−8)		98030.266 (−43)
7	98349.513 (12)	98269.333 (*)	98197.924 (−38)	98209.794 (82)		98054.206 (−7)
8	98379.587 (−9)	98298.890	98226.549 (−70)	98238.590 (*)		98081.578 (30)
9	98413.415 (56)	98331.716	98258.699 (−71)	98270.759 (−81)		98112.243 (44)
10	98450.886 (37)	98368.526	98294.361 (*)	98306.531 (55)		98146.620 (6)
11	98492.133 (15)	98408.701	98333.946	98346.621 (*)		98184.062 (46)
12	98537.080 (−27)	98454.314	98377.064	98389.229		98225.166 (92)
13	98585.779 (76)			98436.105		98269.547 (*)
14	98638.200 (−43)			98486.598		98317.396 (58)
15	98694.538 (67)					98368.494 (−65)
16	98754.504 (*)					98422.903
17	98818.246 (91)					
18	98885.902 (*)					
19	98956.419 (14)					
20	99031.355 (34)					
21	99109.060					

Notes. See note to Table A.11.

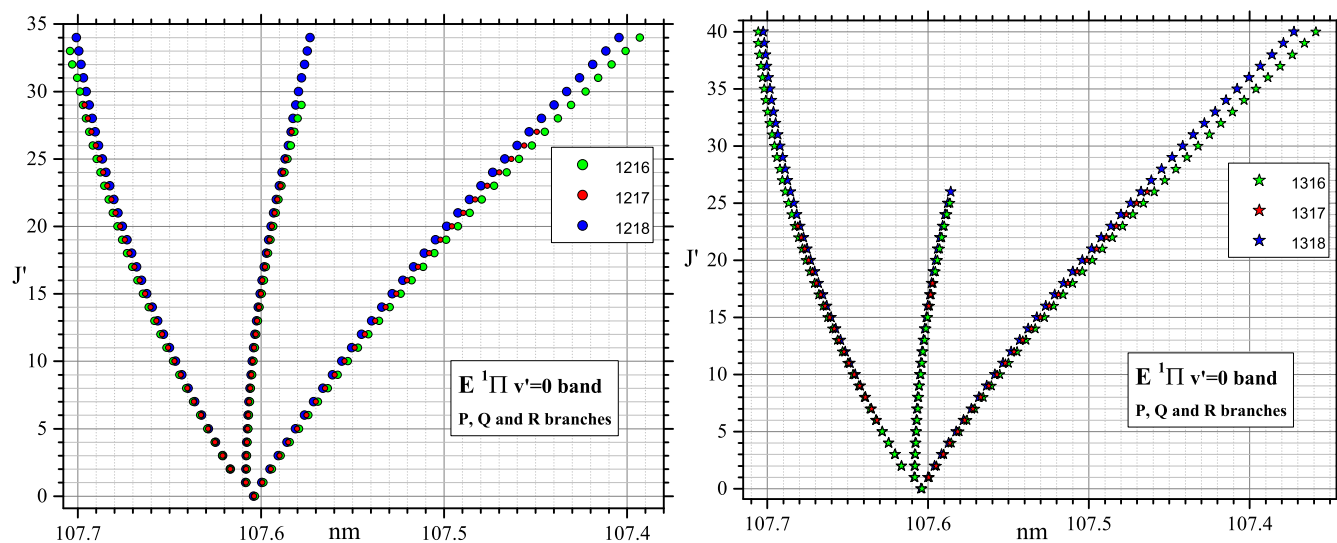


Fig. A.12. Transition wavelengths of the $E^1\Pi(v'=0)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

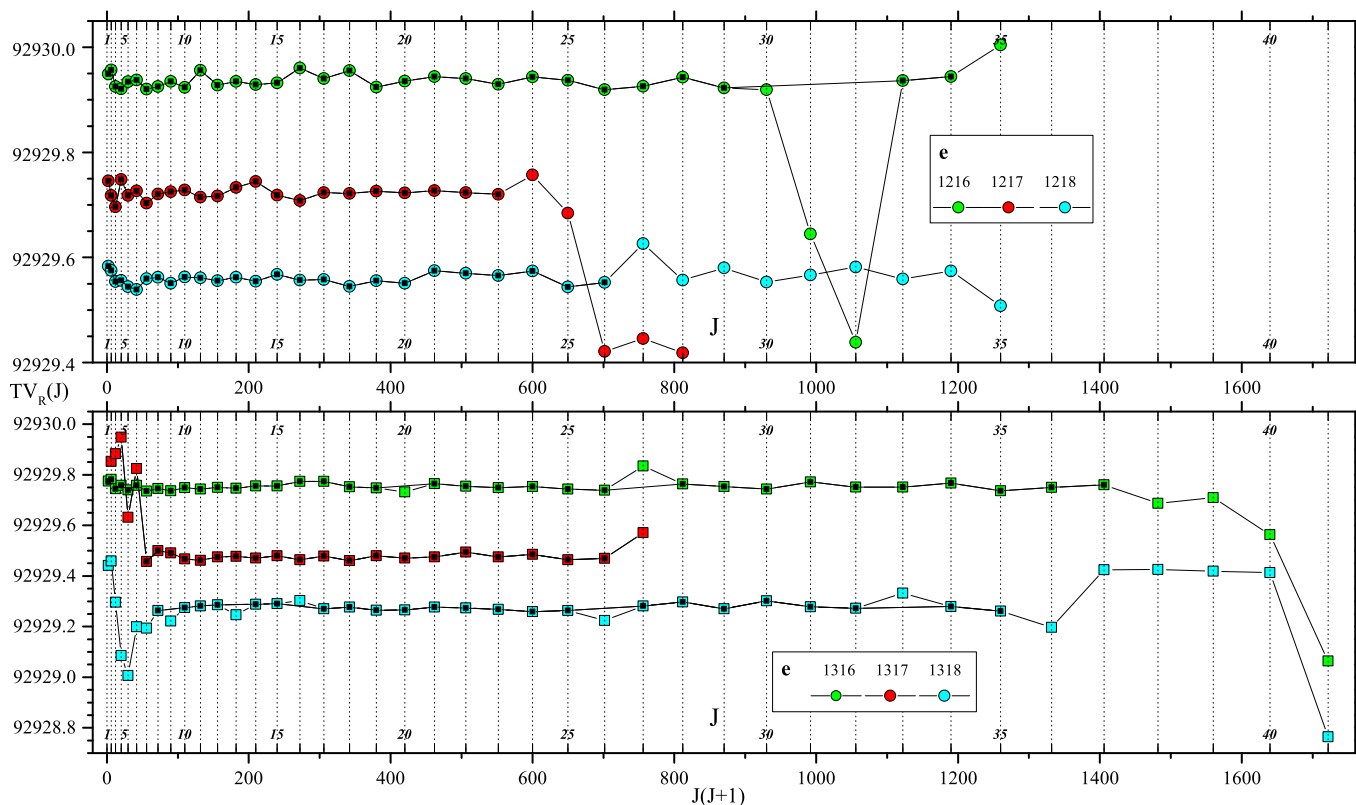


Fig. A.13. e -parity reduced term values (cm^{-1}) of the $E^1\Pi(v'=0)$ levels for six CO isotopologues. Data marked with a black center are kept to calculate molecular constants.

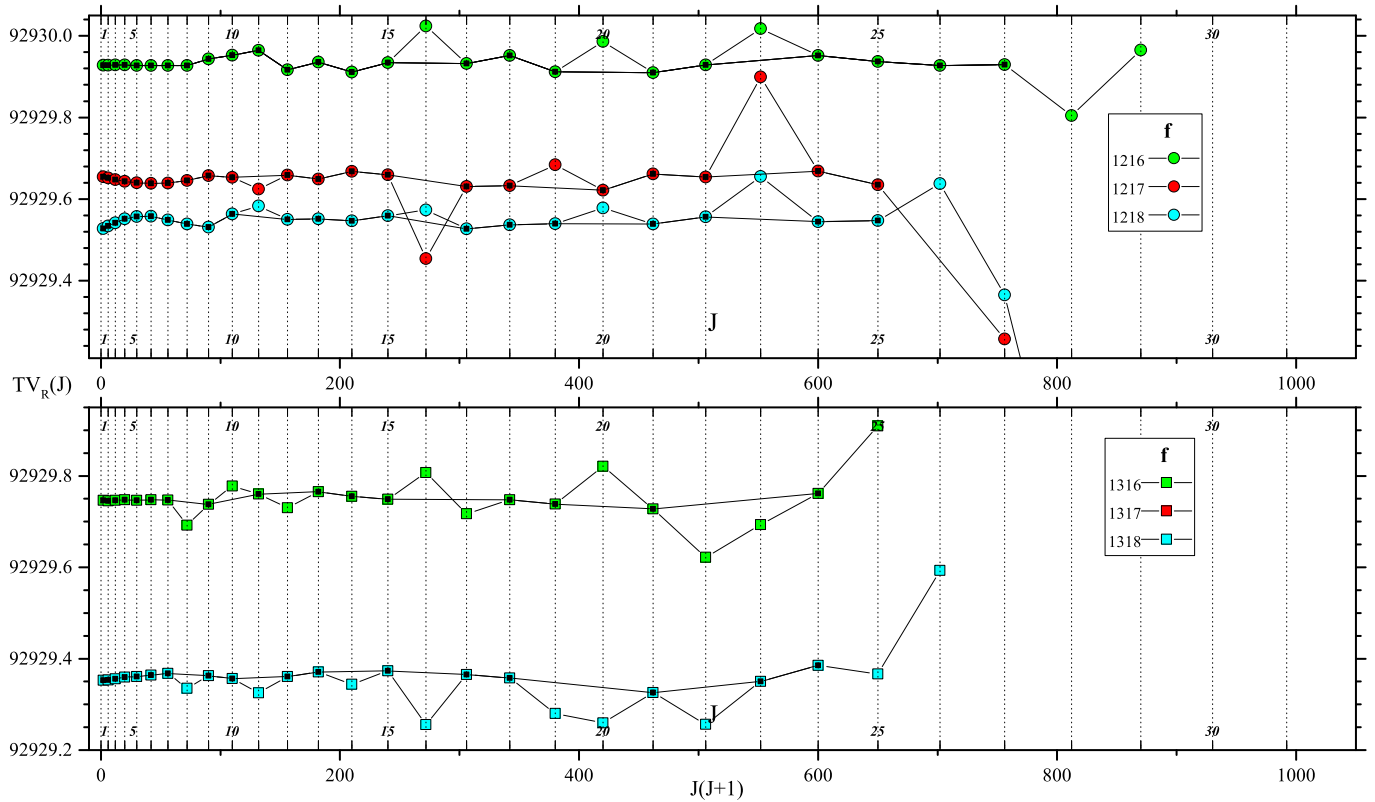


Fig. A.14. f -parity reduced term values (cm^{-1}) of the $E^1\Pi(v'=0)$ levels for six CO isotopologues (data marked with a black center are kept to calculate molecular constants).

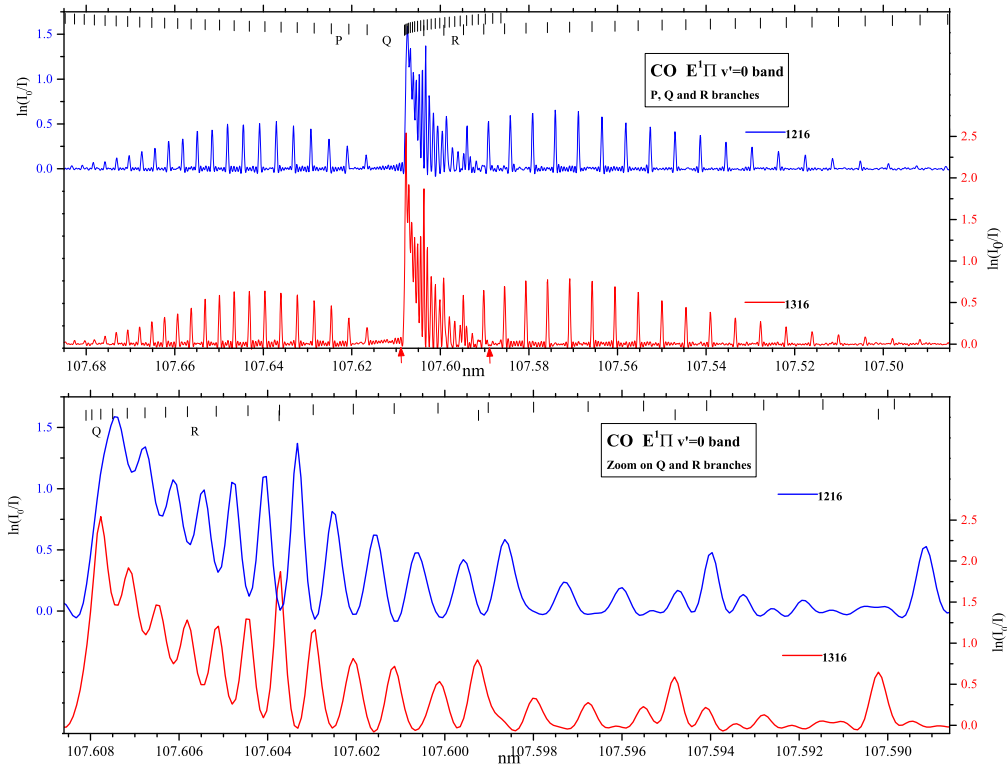


Fig. A.15. Spectra of the $E^1\Pi(v'=0)$ – $X^1\Sigma^+(v''=0)$ band for $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{16}\text{O}$. The lower graph shows a $\times 10$ expanded scale on the Q -branch (between the red arrows).

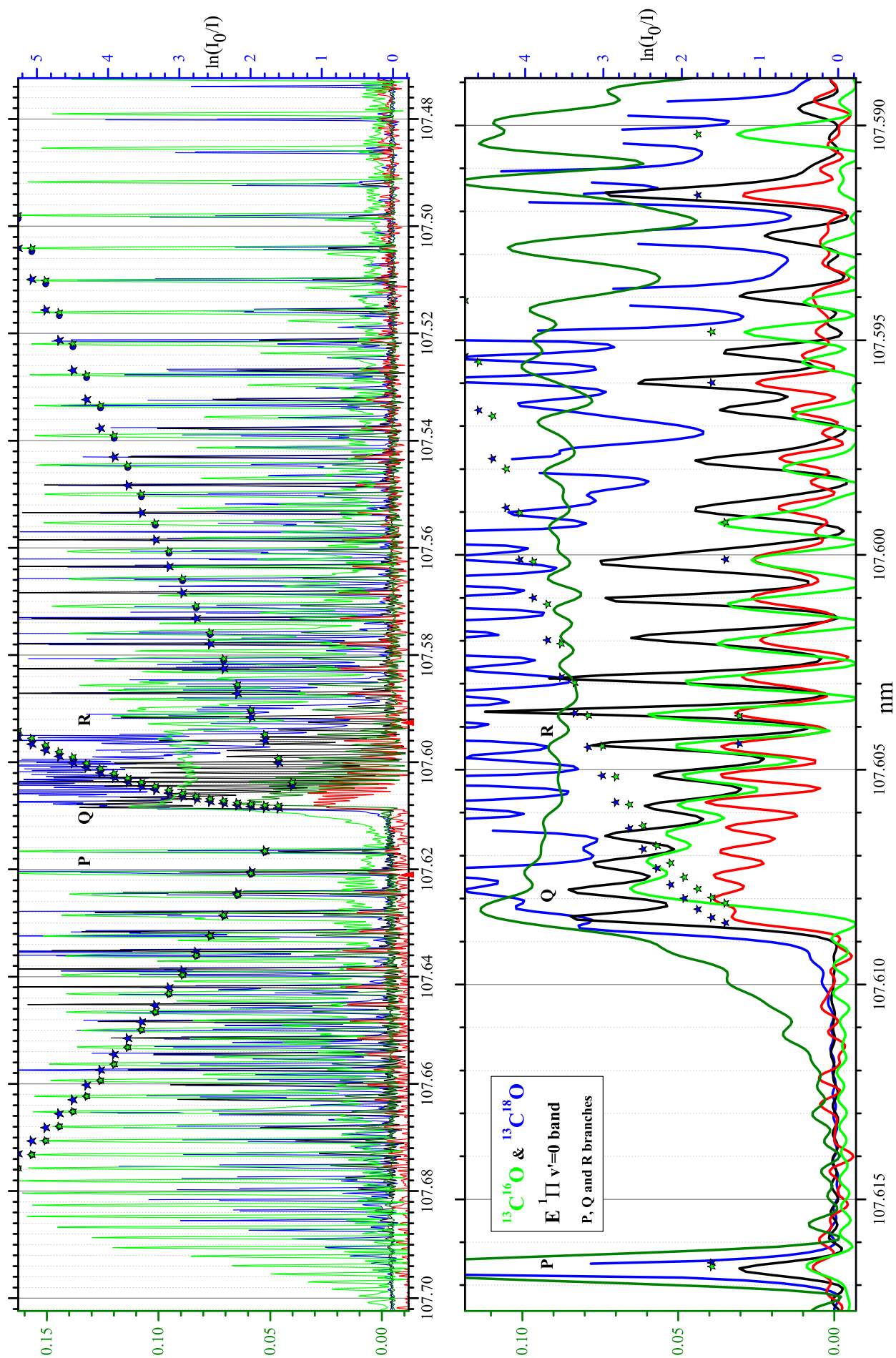


Fig. A.16. *Top:* spectra of the $E' \Pi(v' = 0) - X' \Sigma^+(v' = 0)$ band for $^{13}\text{C}^{18}\text{O}$ (three spectra at different pressures [saturated, half saturated, and no saturation]: 0.5/0.03/0.004 mbar, respectively, in blue/black/red colors; the scale to the right is valid for the highest pressure and has to be divided by 2 and 10 for the latter ones) and $^{13}\text{C}^{16}\text{O}$ (two spectra [saturated and no saturation]: 0.5/0.005 mbar respectively in olive/green colors; the scale to the left is the same for both pressures). *Bottom:* this is an x8 expanded scale on the Q-branch between the red arrows (same color codes and same relative scales as above).

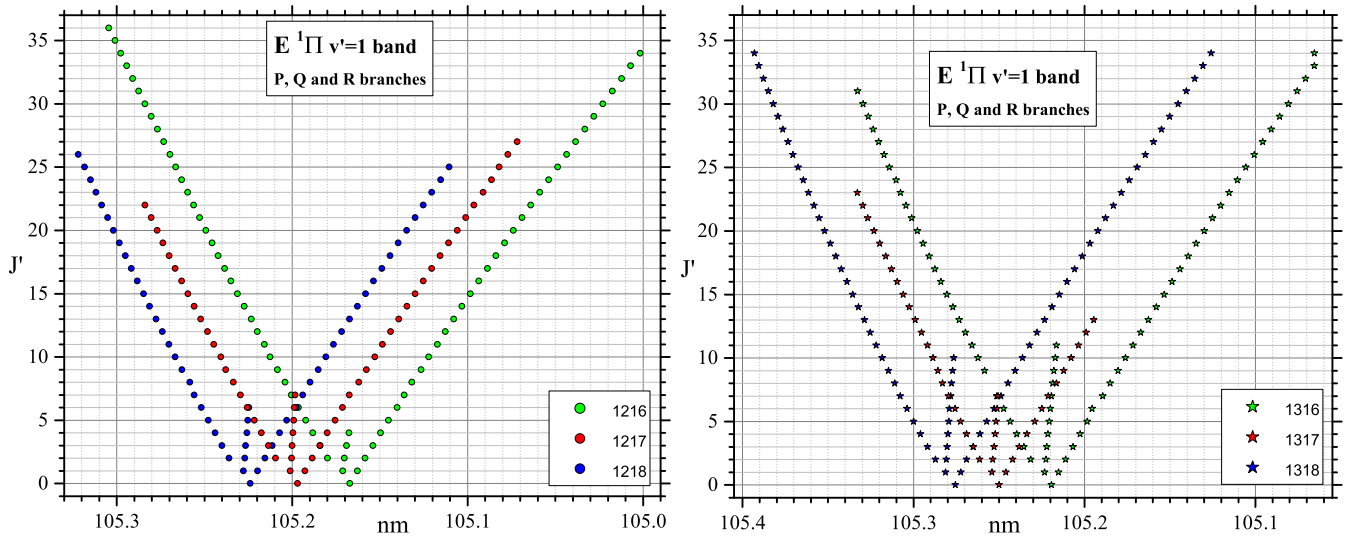


Fig. A.17. Transition wavelengths of the $E^1\Pi(v'=1)-X^1\Sigma^+(v''=0)$ band for six CO isotopologues.

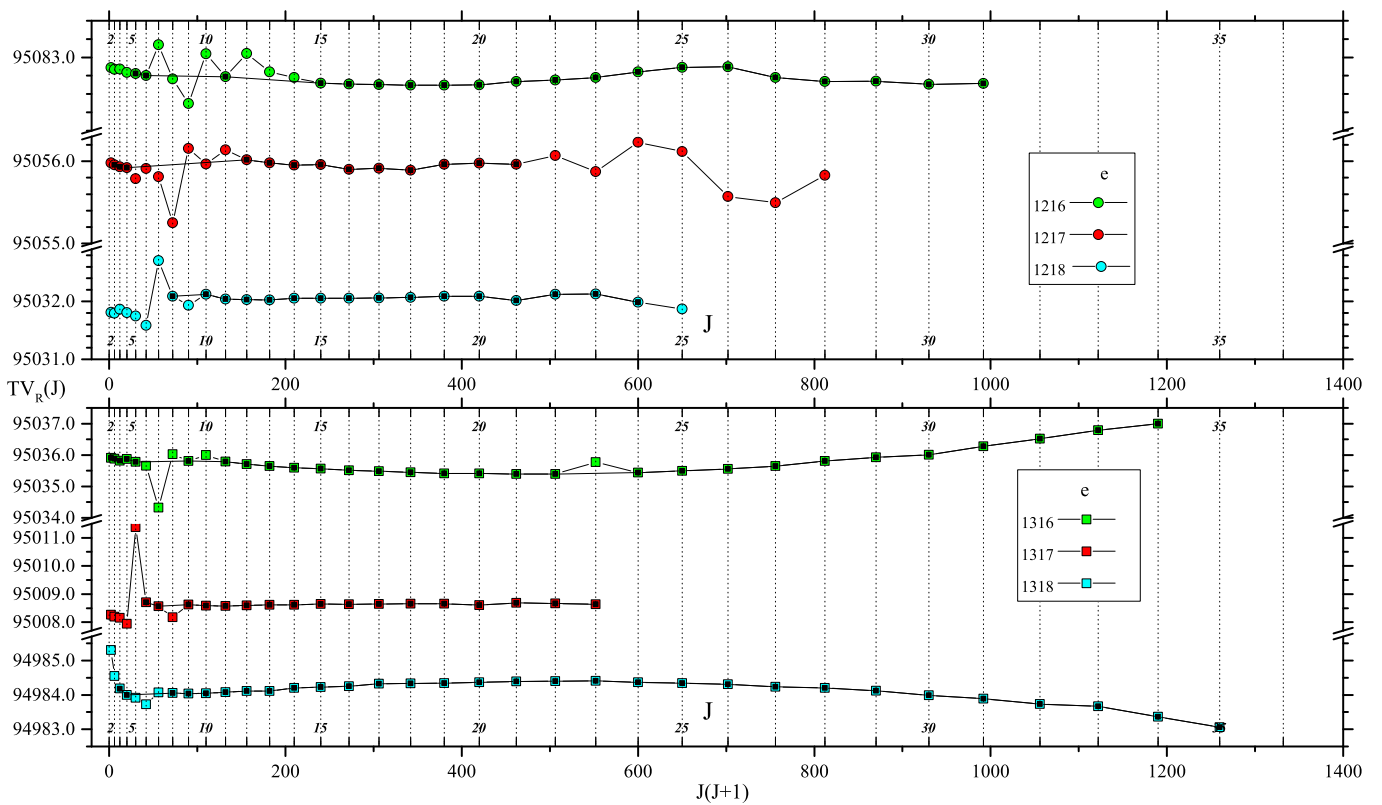


Fig. A.18. e -parity reduced term values (cm^{-1}) of the $E^1\Pi(v'=1)$ levels for six CO isotopologues (left). Data marked with a black center are kept to calculate molecular constants.

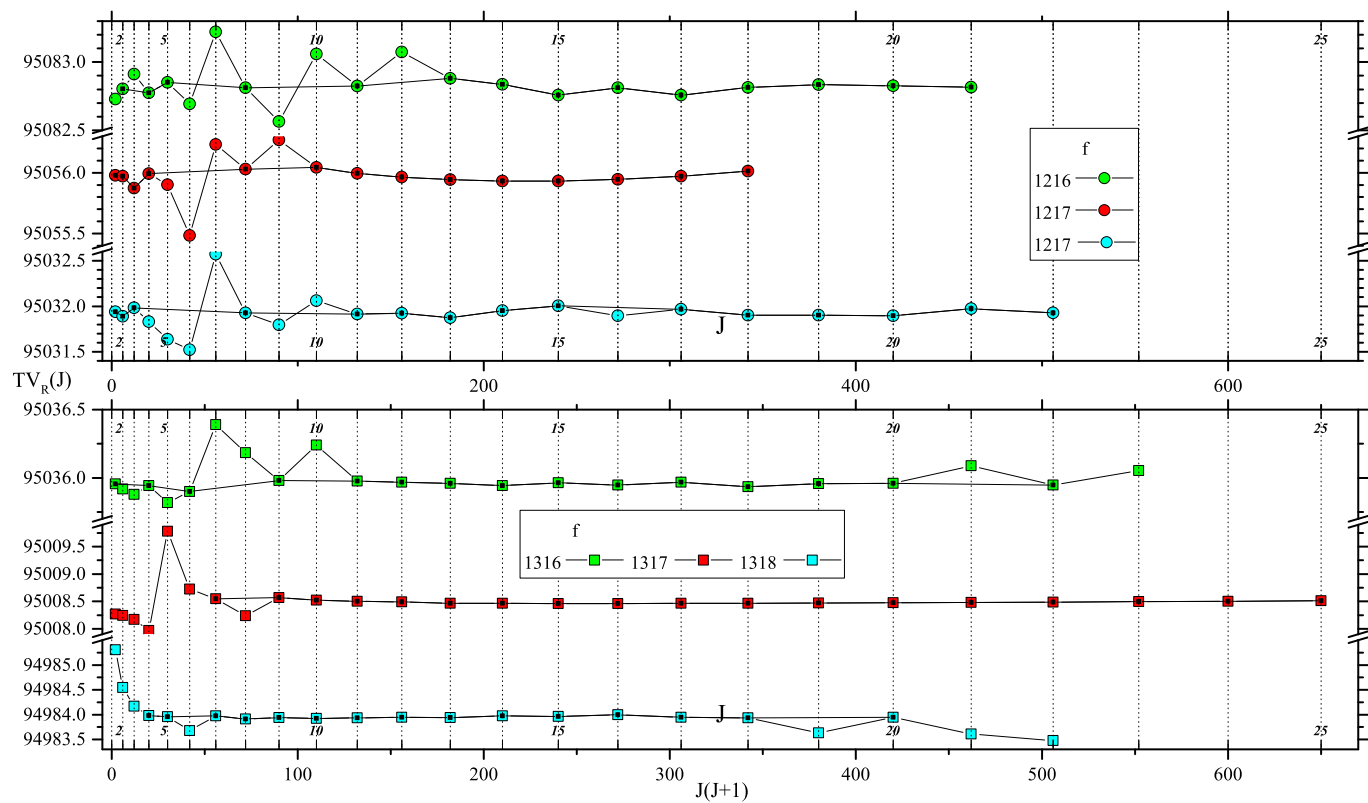


Fig. A.19. f -parity reduced term values (cm^{-1}) of the $E^1\Pi(v' = 1)$ levels for six CO isotopologues (data marked with a black center are kept to calculate molecular constants).

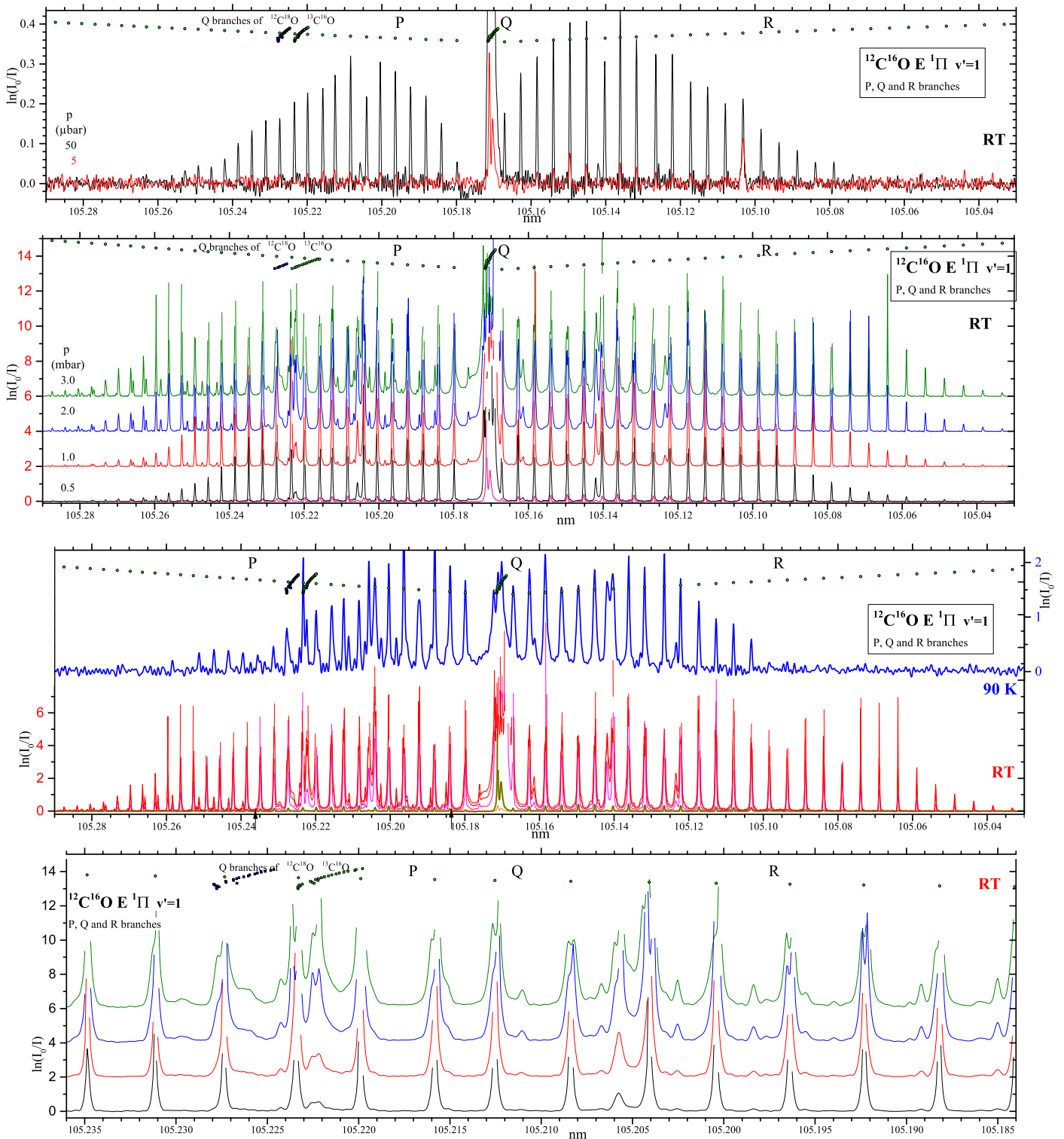


Fig. A.20. Spectra of the $E^1\Pi(v'=1)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{16}\text{O}$. *Two upper panels:* RT spectra taken at different pressures. *Third panel:* comparison between 90 K (1 pressure) and room-temperature spectra (all pressures). *Lower panel:* $\times 5$ expanded scale on the region indicated by black arrows on the above panel. This region contains among other lines those of the $k^3\Pi(v'=5)$ perturbing band (around 105.205 nm), while $k^3\Pi(v'=6)$ appears around 105.14 nm.

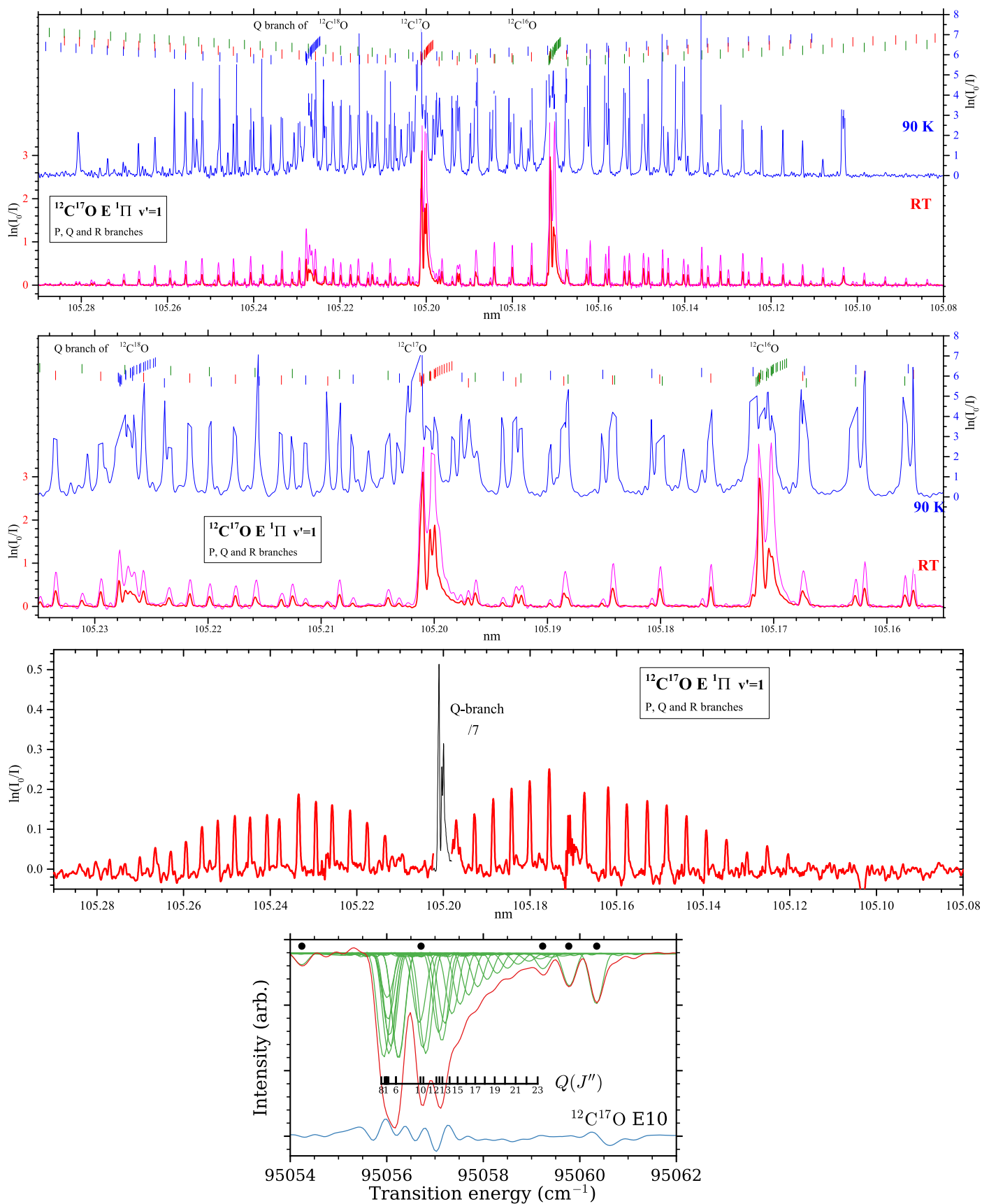


Fig. A.21. Spectra of the $E^1\Pi(v'=1)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{17}\text{O}$ at 90 K and at room temperature (two pressures for the latter). *Second panel:* zoom of the central part of the *upper panel* ($\times 3$ zoom). *Third panel:* RT spectrum after weighted subtraction of $^{12}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ spectra (the signal in the *Q*-branch, in black, is divided by 7). *Lower panel:* simulated absorption spectrum of the *Q*-branch at room temperature.

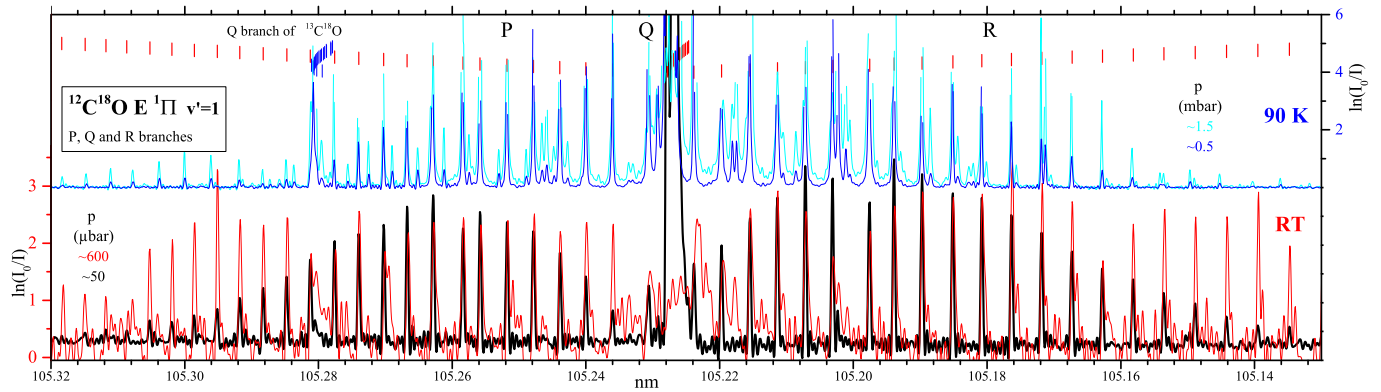


Fig. A.22. Spectra of the $E^1\Pi(v' = 1) - X^1\Sigma^+(v'' = 0)$ band for $^{12}\text{C}^{18}\text{O}$ at 90 K and room temperature (both at two pressures).

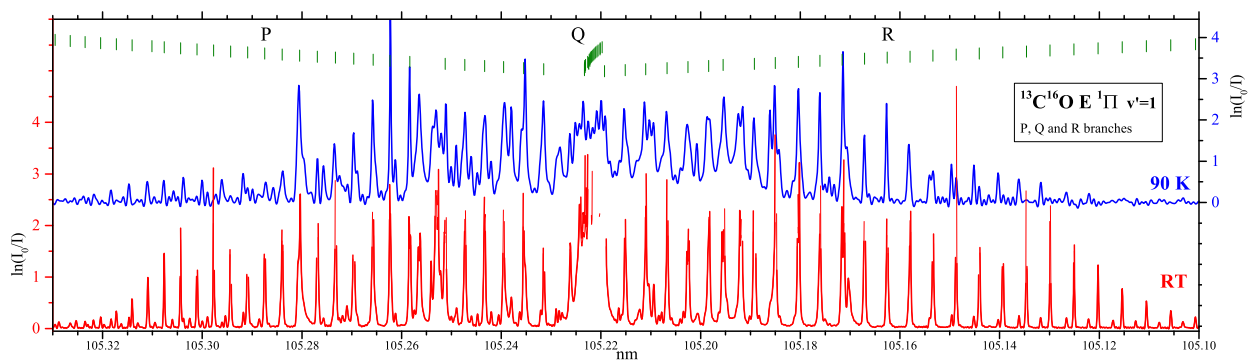


Fig. A.23. Spectra of the $E^1\Pi(v' = 1) - X^1\Sigma^+(v'' = 0)$ band for $^{13}\text{C}^{16}\text{O}$ at 90 K and room temperature.

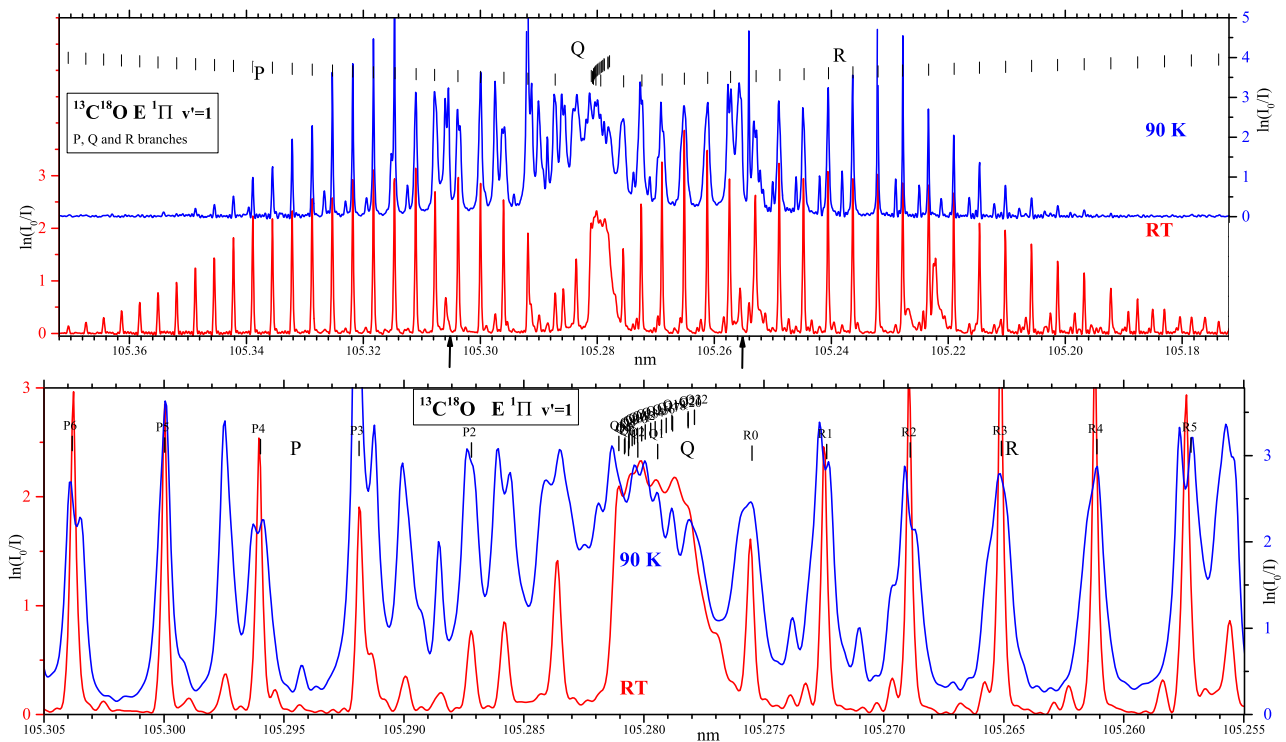


Fig. A.24. Upper panel: spectra of the $E^1\Pi(v' = 1) - X^1\Sigma^+(v'' = 0)$ band for $^{13}\text{C}^{18}\text{O}$ at 90 K and room temperature. Lower panel: $\times 4$ expanded scale on the Q-branch between the black arrows.

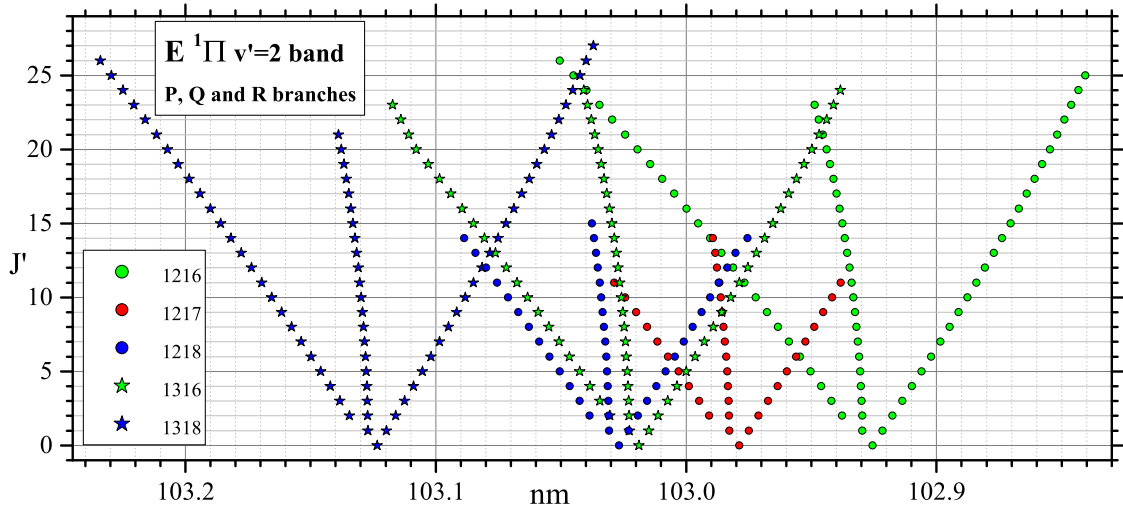


Fig. A.25. Transition wavelengths of the $E^1\Pi(v'=2)-X^1\Sigma^+(v''=0)$ band for five CO isotopologues.

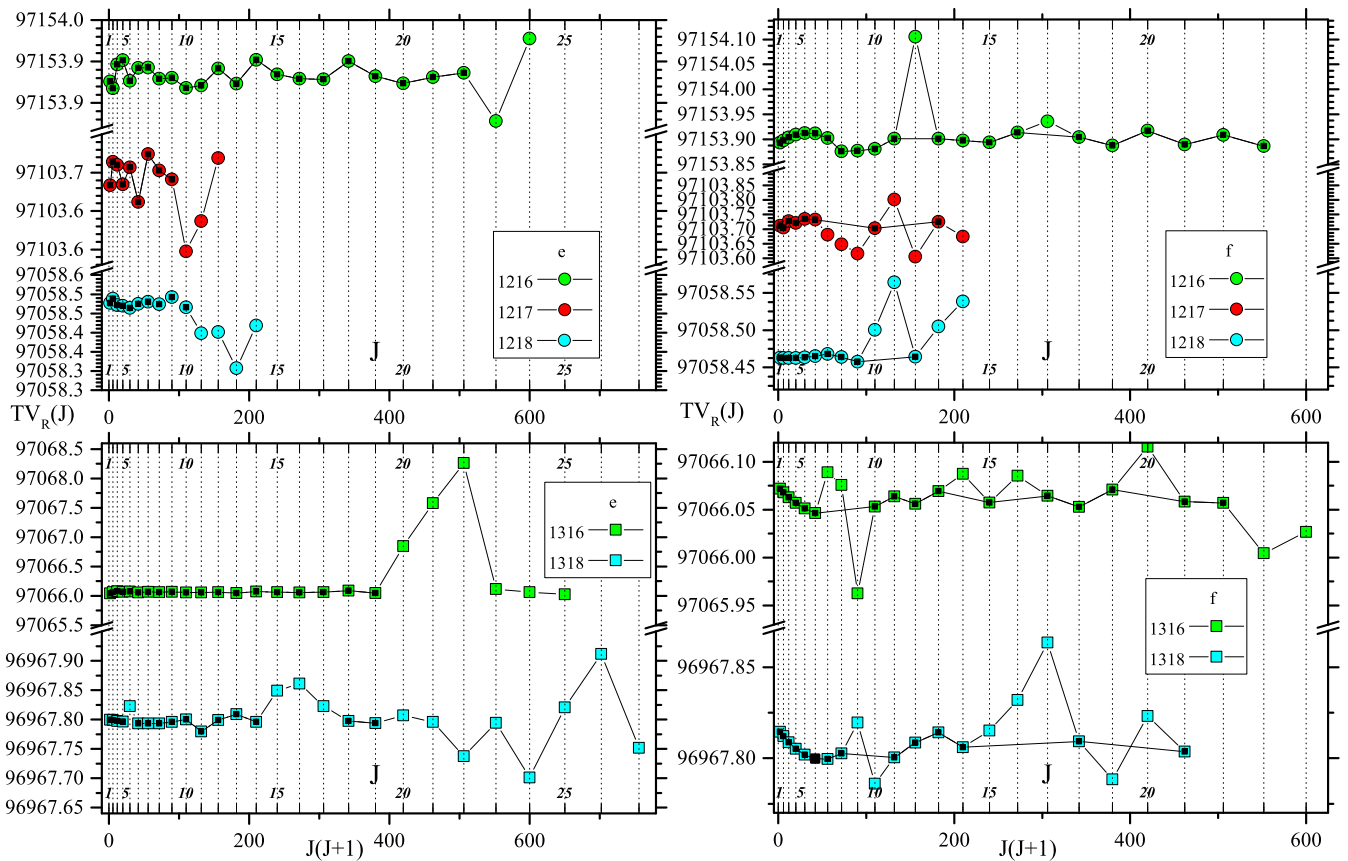


Fig. A.26. Reduced term values (cm^{-1}) of the $E^1\Pi(v'=2)$ levels for five CO isotopologues (left: e -parity and right: f -parity). Data marked with a black center are kept to calculate molecular constants.

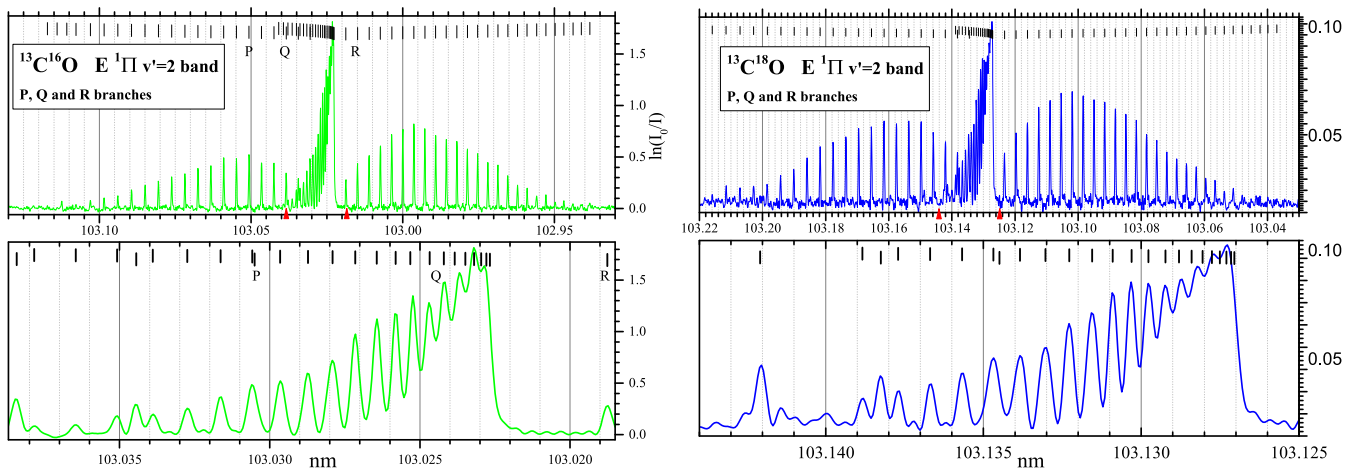
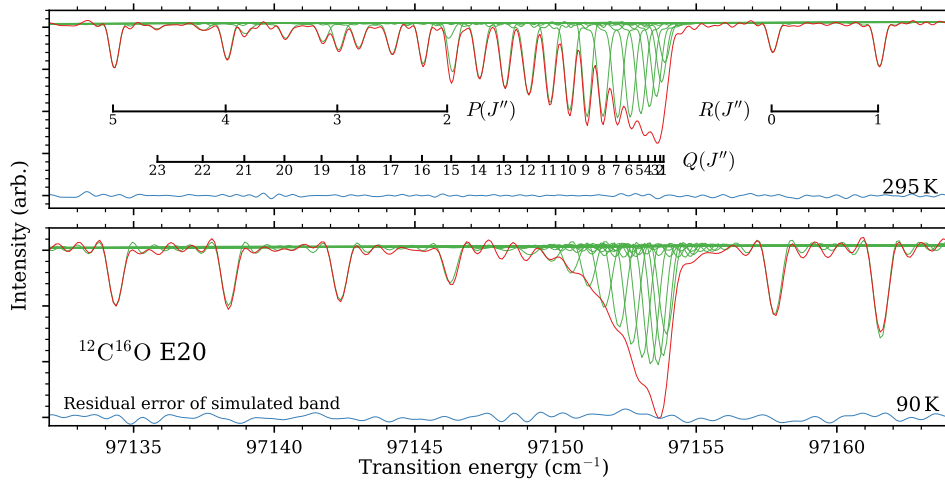


Fig. A.27. Spectra of the $E^1\Pi(v'=2)-X^1\Sigma^+(v''=0)$ band. *Upper panel:* Simulated absorption spectra of the Q -branch of the for $^{12}\text{C}^{16}\text{O}$ at 90 K and at room temperature. *Lower panels:* spectra of $^{13}\text{C}^{16}\text{O}$ (left) and $^{13}\text{C}^{18}\text{O}$ (right). *Lowest panel:* $\times 10$ expanded scale on the Q -branch (between the red arrows).

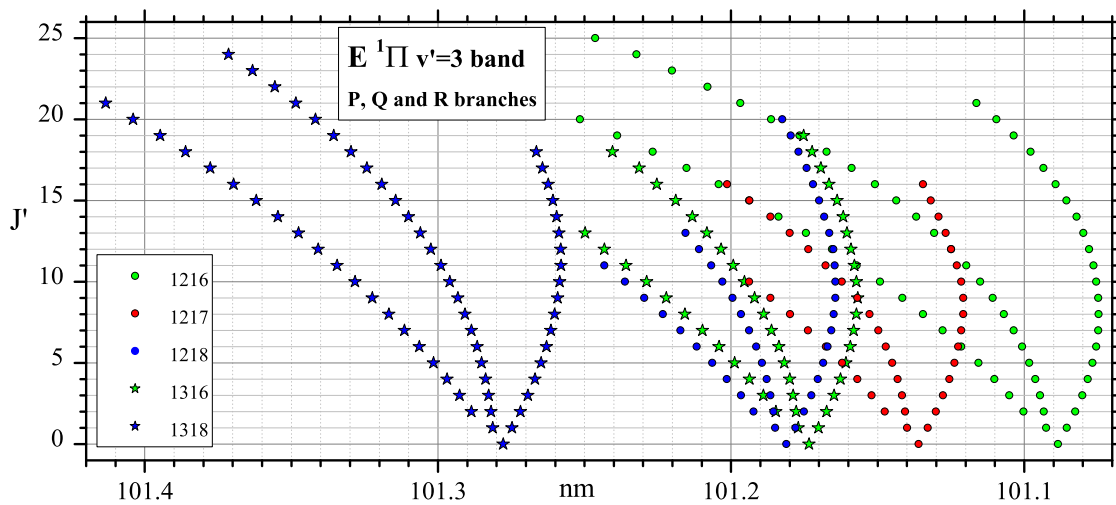


Fig. A.28. Transition wavelengths of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for the five observed CO isotopologues.

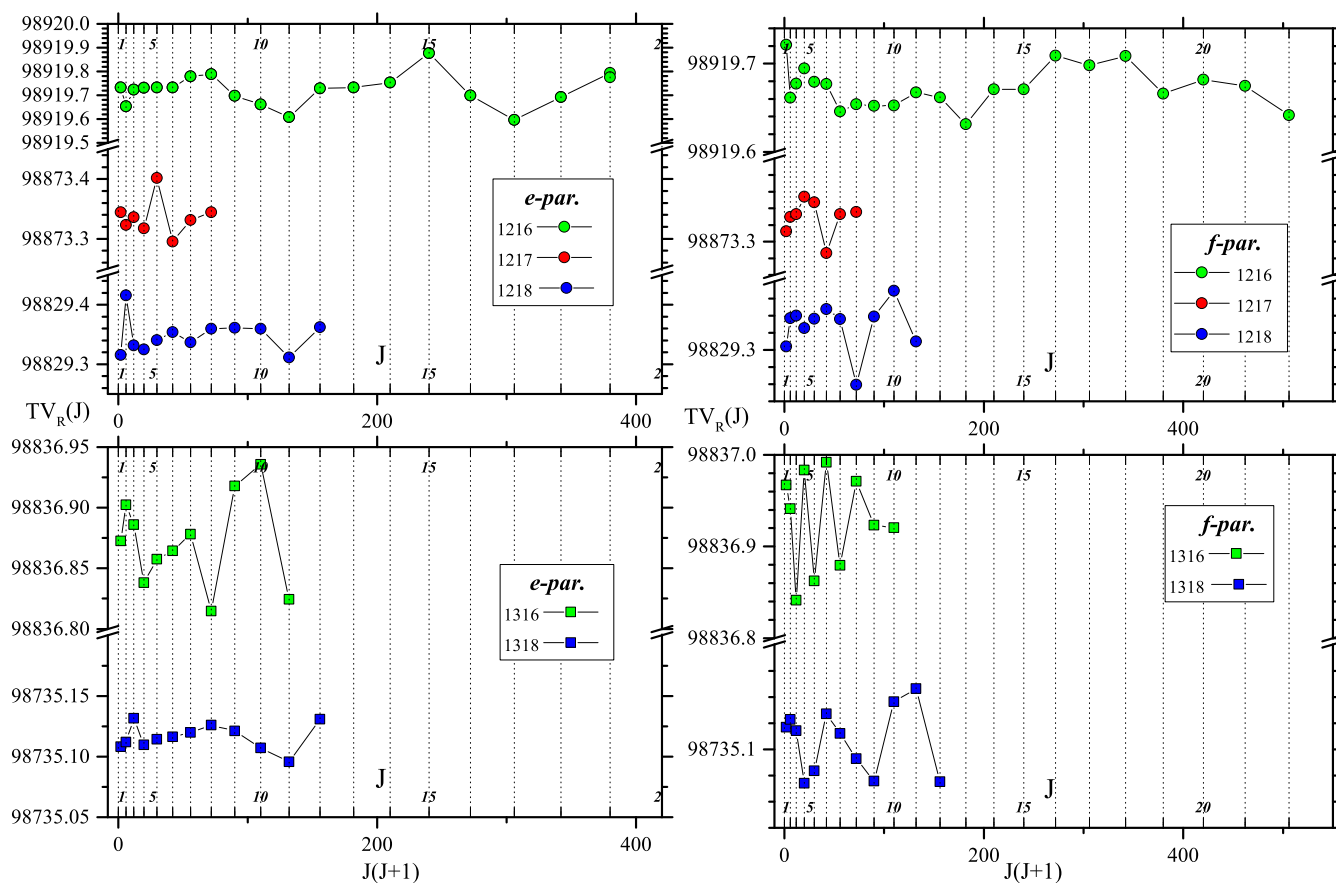


Fig. A.29. Reduced term values (cm^{-1}) of the $E^1\Pi(v'=3)$ levels for the five observed CO isotopologues (left: e -parity, and right: f -parity).

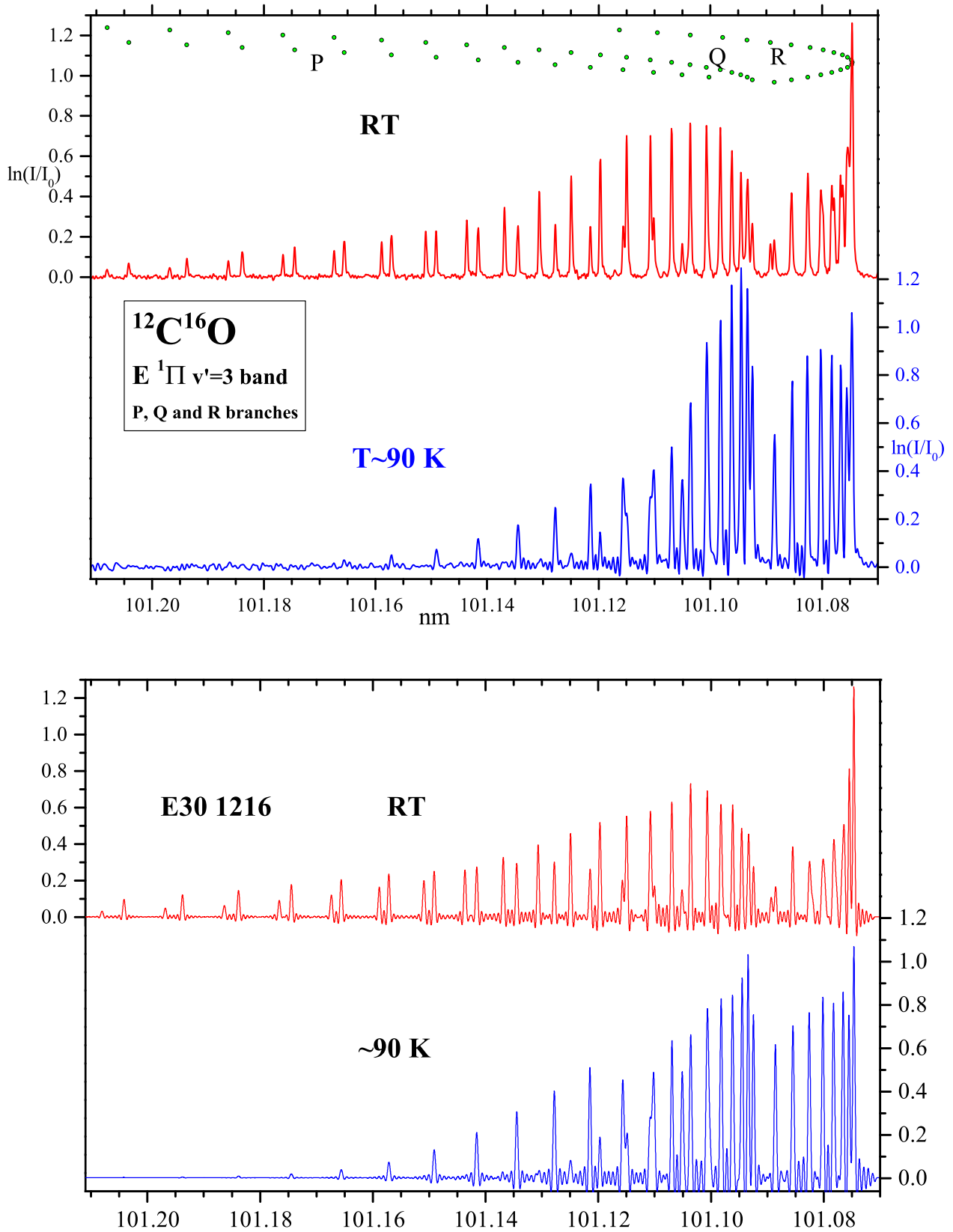


Fig. A.30. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{16}\text{O}$ at room temperature (RT) and at ~ 90 K. Simulations below, in emission, of the upper experimental spectra (using classical Hönl–London factors).

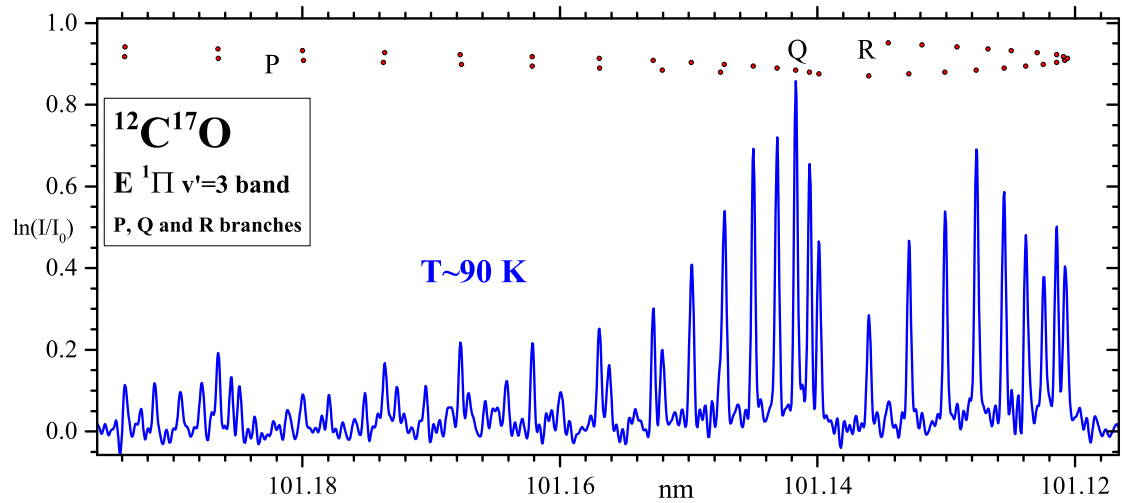


Fig. A.31. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{17}\text{O}$ at ~ 90 K. Traces of $^{12}\text{C}^{18}\text{O}$ are present around 101.185 nm.

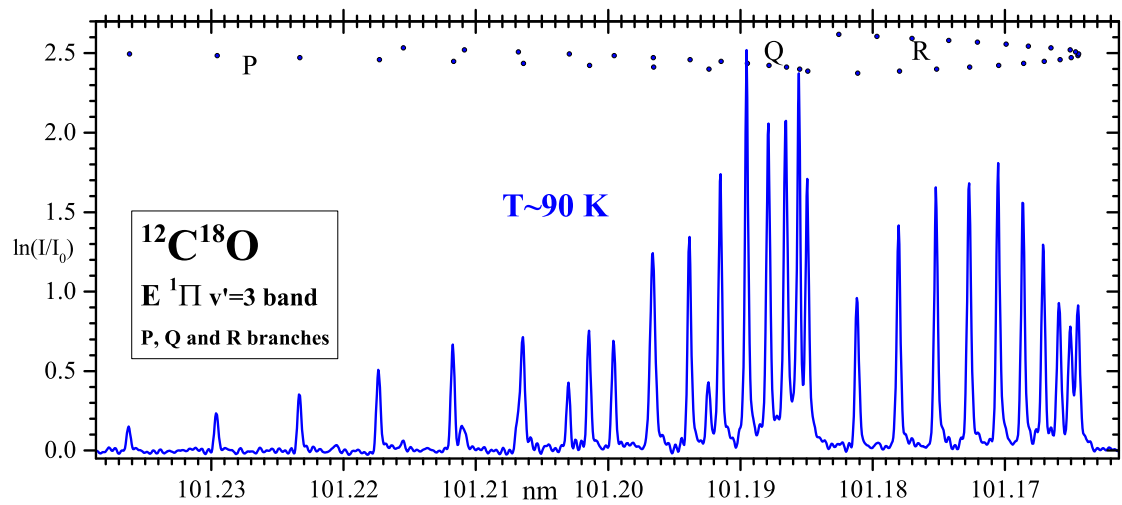


Fig. A.32. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{18}\text{O}$ at ~ 90 K.

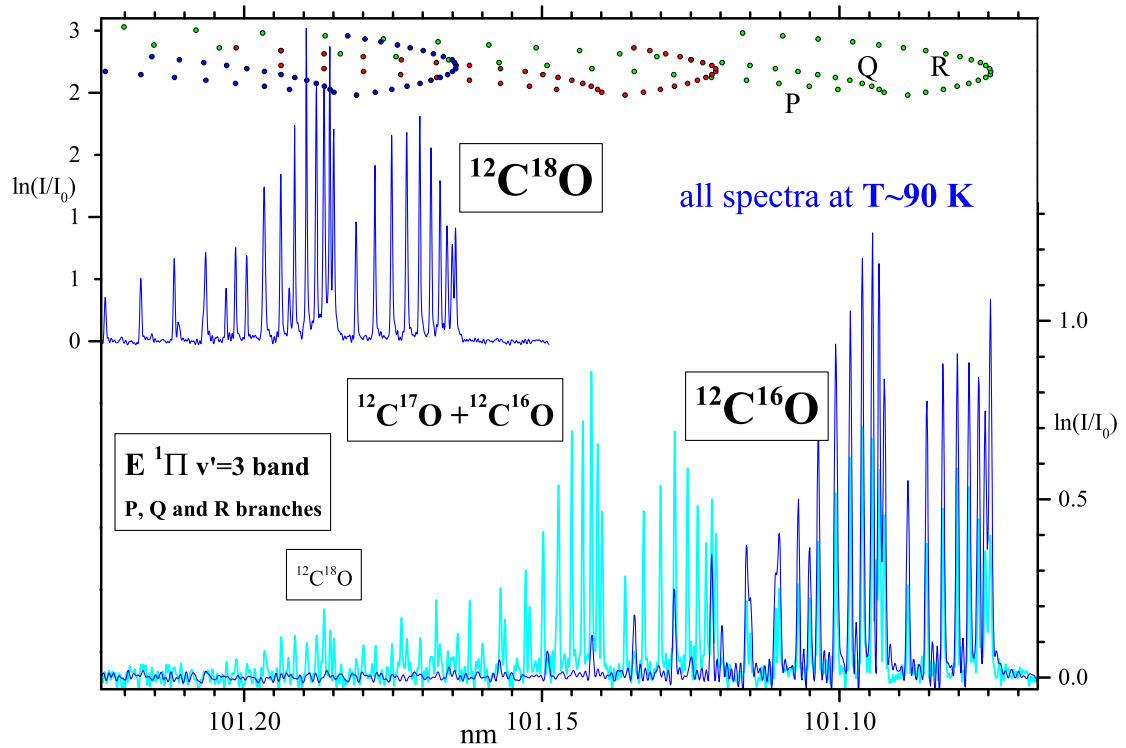


Fig. A.33. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, and $^{12}\text{C}^{18}\text{O}$ at ~ 90 K. $^{12}\text{C}^{17}\text{O}$ is about equally mixed with $^{12}\text{C}^{16}\text{O}$, and traces of $^{12}\text{C}^{18}\text{O}$ are present.

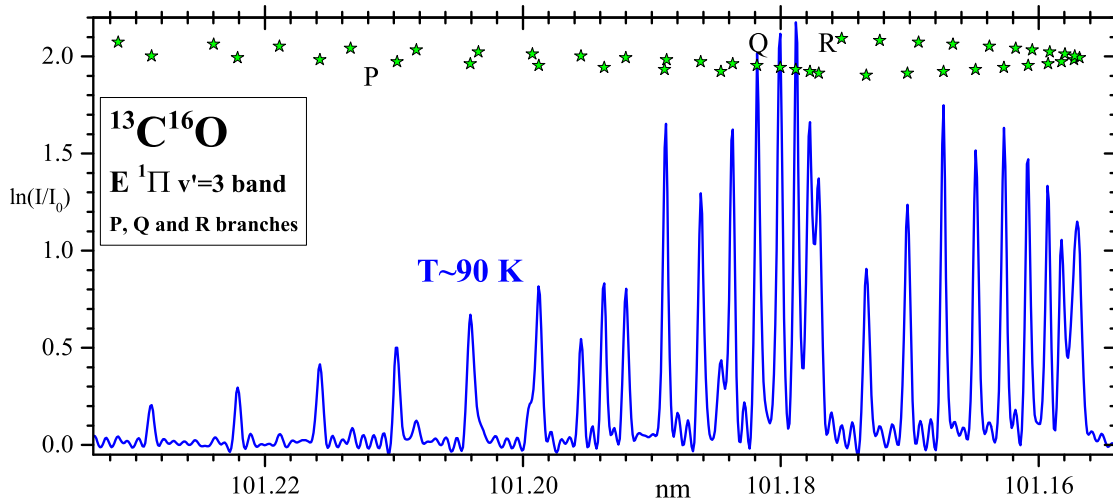


Fig. A.34. Spectrum of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{13}\text{C}^{16}\text{O}$ at ~ 90 K.

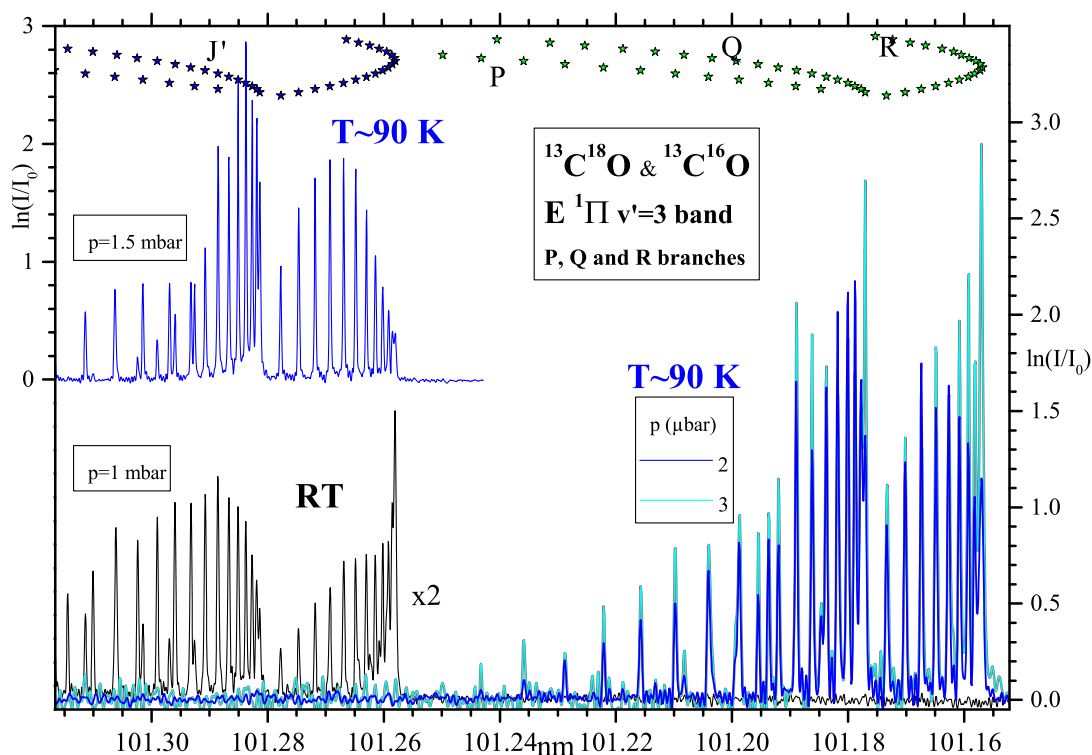


Fig. A.35. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{13}\text{C}^{16}\text{O}$ at ~ 90 K (at two pressures) and $^{13}\text{C}^{18}\text{O}$ at room temperature (in black) and ~ 90 K (with two different blues).

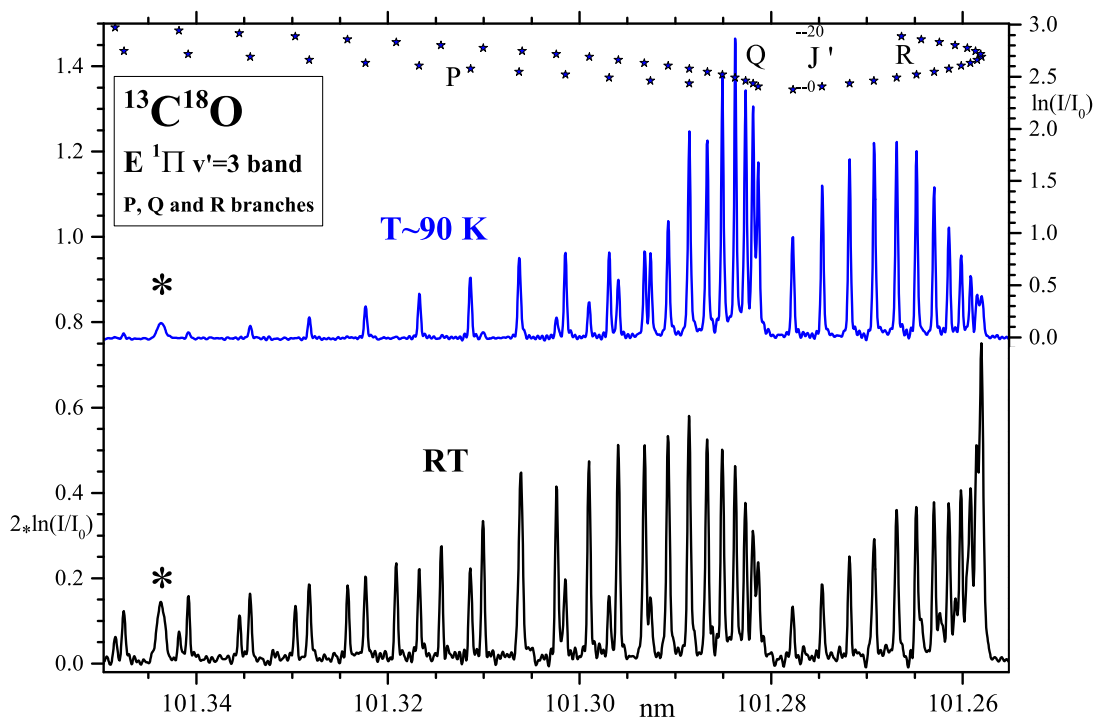


Fig. A.36. Spectra of the $E^1\Pi(v'=3)-X^1\Sigma^+(v''=0)$ band for $^{13}\text{C}^{18}\text{O}$ at room temperature (RT) and at ~ 90 K. The asterisk shows an impurity line in the gas filter.

Table A.21. Term values (cm^{-1}) of the $E^1\Pi(v''=0)$ e - and f -parity levels for six CO isotopologues.

J'	$^{12}\text{C}^{16}\text{O}$			$^{12}\text{C}^{17}\text{O}$			$^{13}\text{C}^{16}\text{O}$			$^{13}\text{C}^{17}\text{O}$		
	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J
1	92933.878 (30)	92933.833 ^a	0.045	92933.462 ^a	92933.247 ^a	0.077	92933.325 (27)	92933.486 ^a	0.050	92941.048 (68)	92940.940 ^a	0.102
2	92941.744 (55)	92941.644 ^a	0.100	92941.075 ^a	92940.692 ^a	0.106	92940.798 (55)	92940.946 ^a	0.102	92951.820	92951.900 ^a	0.110
3	92953.499 (12)	92953.360 ^a	0.139	92952.673 (40)	92952.493 ^a	0.180	92952.76 (27)	92952.147 ^a	0.129	92951.820	92951.900 ^a	0.168
4	92969.209 (17)	92968.980 ^a	0.229	92967.718 ^a	92966.743 ^a	0.221	92967.309 (-13)	92967.080 ^a	0.229	92964.762 (7)	92964.828 ^a	0.066
5	92988.865 (-1)	92988.502 ^a	0.363	92987.156 (1)	92986.750 ^a	0.406	92986.665 (-2)	92985.343 ^a	0.311	92984.470 (7)	92984.563 ^a	-0.043
6	93012.438 (-6)	93011.929 ^a	0.508	93010.137 (2)	93009.589 ^a	0.547	93008.091 (0)	93008.141 ^a	0.469	93006.594 (7)	93003.844 ^a	0.271
7	93039.915 (4)	93039.258 ^a	0.657	93036.912 (19)	93036.235 ^a	0.677	93034.867 (-3)	93033.675 ^a	0.616	93031.813 (121)	93028.671 ^a	0.406
8	93071.339 (3)	93070.488 ^a	0.851	93067.553 (1)	93066.689 ^a	0.863	93064.290 (-5)	93063.409 ^a	0.800	93061.093 (-56)	93057.006	0.674
9	93145.946 (-6)	93145.634	1.058	93140.279 (-15)	93138.997	1.284	93135.249 (-9)	93134.063	1.186	93130.972 (-36)	93128.945	0.788
10	93189.164 (-1)	93187.609	1.555	93182.357 (-10)	93180.817	1.540	93176.368 (-8)	93174.965	1.403	93170.487 (-12)	93163.355	1.312
11	93236.240 (-19)	93234.382	1.858	93228.270 (-11)	93226.498	1.773	93221.214 (-11)	93219.526	1.688	93214.514 (12)	93205.926	1.523
12	93287.268 (-7)	93285.114	2.154	93278.016 (-3)	93275.929	2.087	93269.803 (-2)	93269.325	1.964	93261.994 (-4)	93252.010	1.733
13	93342.190 (-4)	93339.694	2.504	93331.572 (-1)	93329.181	2.391	93323.807 (0)	93321.522	2.283	93313.108 (1)	93301.595	2.079
14	93401.050 (-4)	93398.212	2.839	93388.904 (2)	93386.198	2.707	93378.135 (11)	93377.444	2.617	93367.880 (3)	93354.773	2.348
15	93463.838 (-5)	93460.682	3.156	93450.064 (-2)	93446.804	3.260	93437.905 (1)	93437.142	2.922	93426.266 (-2)	93411.338	2.793
16	93530.484 (-5)	93526.855	3.629	93511.579	93509.962	3.479	93501.388 (4)	93498.062	3.326	93488.318 (-1)	93471.663	2.980
17	93601.072 (-3)	93597.021	4.050	93583.842 (-2)	93579.962	3.880	93568.577 (-9)	93564.887	3.690	93553.973 (15)	93535.404	3.340
18	93675.514 (15)	93671.007	4.507	93652.174	93652.174	4.261	93639.506 (3)	93635.401	4.105	93623.295 (8)	93602.603	3.768
19	93753.899 (18)	93748.983	4.916	93728.089	93728.089	4.773	93714.135 (1)	93709.645	4.490	93696.218 (2)	93677.553 (11)	4.166
20	93836.178 (-2)	93830.681	5.496	93807.799	93807.799	5.214	93792.503 (-4)	93787.501	5.002	93772.782 (-16)	93747.784	4.503
21	93922.337 (6)	93916.344	5.993	93891.273	93891.273	5.719	93874.551 (-8)	93869.101	5.450	93852.983 (-22)	93825.568	4.973
22	94012.379 (-13)	94005.944	6.435	93986.992 (21)	93986.992	6.197	93964.305 (-11)	93954.467	5.838	93936.765	93907.037	5.292
23	94106.331 (-14)	94096.467	7.081	94076.360 (-33)	94069.544	6.816	94049.774 (-3)	94043.304	6.696	94024.193	93991.966	5.679
24	94204.145 (1)	94192.500	7.682	94171.633 (21)	94164.280	7.353	94142.903 (-5)	94135.934	6.979	94115.203	94080.358	6.144
25	94305.826 (-5)	94297.544	8.282	94270.495 (7)	94264.069	7.953	94239.766 (-1)	94232.325	7.441	94209.849	94172.509	6.332
26	94411.406 (9)	94402.485	8.921	94373.422 (7)	94364.698	8.723	94340.385 (-8)	94332.024	8.361	94324.798 (14)	94274.730 (-6)	6.332
27	94520.866 (2)	94511.144	9.722	94480.069 (7)	94472.500	9.540	94444.530 (0)	94435.010	9.360	94424.954 (6)	94374.230 (-6)	6.332
28	94634.154 (8)	94623.932	10.222	94552.491 (-4)	94545.928	10.563	94524.919 (-4)	94515.928	10.363	94505.537 (5)	94477.134 (6)	6.332
29	94751.320 (-8)	94742.072 (7)	11.491	94664.061 (-7)	94652.570	11.491	94640.867 (14)	94636.606 (-2)	11.491	94623.983 (58)	94583.607 (6)	6.332
30	94872.072 (7)	94862.538	12.473	94779.347 (3)	94776.874	12.473	94766.606 (-2)	94760.874	12.473	94751.320 (-8)	94693.532 (-1)	6.332
31	94996.743 (7)	94987.182	13.455	94898.307 (-17)	94893.307	13.455	94883.307 (-17)	94878.307	13.455	94864.061 (-7)	94806.976 (11)	6.332
32	95125.965	95116.414	14.437	95020.894 (33)	95015.894	14.437	95005.057 (-2)	95000.057	14.437	94996.743 (7)	94923.983 (58)	6.332
33	95258.538	95249.000	15.419	95147.182	95142.182	15.419	95132.325	95127.325	15.419	95116.414	95044.372 (0)	6.332
34	95395.000	95385.468	16.401	95277.045	95272.045	16.401	95262.045	95257.045	16.401	95249.000	95168.283 (-8)	6.332
35	95528.000	95518.538	17.383	95404.488	95400.488	17.383	95394.488	95389.488	17.383	95381.538	95295.635 (-60)	6.332
36	95661.538	95652.000	18.365	95531.024	95526.024	18.365	95522.024	95517.024	18.365	95504.488	95426.758 (91)	6.332
37	95795.000	95785.468	19.347	95658.468	95653.468	19.347	95646.468	95641.468	19.347	95629.468	95561.129 (54)	6.332
38	95928.538	95918.962 (93)	20.329	95785.904	95780.904	20.329	95773.904	95768.904	20.329	95756.904	95698.962 (93)	6.332
39	96062.000	96052.468	21.311	95913.348	95908.348	21.311	95901.348	95896.348	21.311	95884.348	95840.259	6.332
40	96195.538	96185.932	22.293	96040.792	96035.792	22.293	96028.792	96023.792	22.293	96011.792	95984.375	6.332
41	96329.000	96319.400	23.275	96168.236	96163.236	23.275	96156.236	96151.236	23.275	96139.236	96030.311	6.332

Notes. The δ_P value in parentheses (in units of the least significant digit) corresponds to the wavenumber correction applied to TV_P and TV_R . There is no value when the term value is derived from a single transition, either R or P . An asterisk indicates when both R - and P -branches are present at high J' , either the potential presence of a perturbing state or that one of the lines shows a larger uncertainty than the other (see also Sect. 2.2.2). Each third column is the $^1\Pi$ state: $\Lambda_J = \text{TV}_{R&P} - \text{TV}_Q$. ^(a) Data from Cacciani & Ubachs (2004). ^(b) Data calculated from the e -parity levels.

Table A.24. Term values (cm^{-1}) of the $E^1\Pi(v''=1)$ e - and f -parity levels for six CO isotopologues (see note to Table A.21).

J'	$^{12}\text{C}^{16}\text{O}$			$^{13}\text{C}^{16}\text{O}$			$^{12}\text{C}^{18}\text{O}$			$^{13}\text{C}^{18}\text{O}$		
	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J	e -par. (R&P)	f -par. (Q)	Λ_J
1	93086.768 (-11)	95086.586 ^b	0.182	95059.764 (-1)	95059.746 ^a	0.017	95035.504 (-15)	95035.615 ^b	-0.119	95039.643 ^b	95011.857 ^a	0.017
2	95094.514 (20)	95094.376 ^b	0.137	95067.304 (-1)	95067.273 ^a	0.031	95042.876 (12)	95042.915 ^b	-0.039	95046.983 ^b	95010.015 ^a	0.008
3	95106.160 (-5)	95106.056 ^b	0.104	95078.626 (-2)	95078.475 ^a	0.151	95054.029 (24)	95054.033 ^b	-0.006	95058.015 ^b	95029.718 ^a	0.087
4	95121.651 (26)	95121.346 ^b	0.305	95093.745 (13)	95093.661 ^a	0.084	95068.743 (2)	95068.583 ^b	0.158	95072.835 ^b	95043.880 ^a	0.153
5	95141.042 (2)	95140.706 ^b	0.335	95112.518 (-4)	95112.401 ^a	0.116	95087.151 (15)	95086.765 ^b	0.386	95091.486 (1)	95063.643 ^a	1.859
6	95164.303 (6)	95163.686 ^b	0.617	95135.330 (-1)	95134.578 ^a	0.752	95109.150 (28)	95108.695 ^b	0.455	95113.365 ^b	95084.128 ^a	0.355
7	95191.799 (69)	95191.206 ^b	0.592	95161.701 (2)	95161.677 ^a	0.024	95136.116 (17)	95135.465 ^b	0.651	95139.296	95109.601 (-1)	0.516
8	95222.462 (19)	95221.640 ^b	0.823	95191.588 ^a	-0.202	0.829	95165.038 (25)	95164.209 ^b	0.829	95169.692 (-9)	95168.967 ^b	0.579
9	95257.105 (-1)	95256.086 ^b	1.019	95226.307 (-7)	95225.695 ^a	0.612	95198.113 (8)	95197.135 ^b	0.978	95202.889 (15)	95170.929 ^a	0.848
10	95296.429 (37)	95295.122 ^b	1.307	95263.914 (7)	95263.088 ^a	0.826	95235.215 (25)	95234.125 ^b	1.090	95240.172 (-28)	95205.972 ^a	1.040
11	95338.833 (-8)	95337.275 ^b	1.557	95305.654 (10)	95304.408 ^a	1.246	95275.736 (11)	95274.368 ^b	1.668	95289.968 (-2)	95246.673 (-2)	1.254
12	95385.603 (-80)	95383.756 ^b	1.847	95350.870 (3)	95349.493 ^a	1.376	95320.011 (-36)	95318.430 ^b	1.581	95325.191 (16)	95288.464 ^a	1.505
13	95435.787 (-9)	95433.653 ^b	2.152	95399.940 (17)	95398.331 ^a	1.609	95367.972 (20)	95366.096 ^b	1.876	95373.330 (8)	95335.075 ^a	1.789
14	95489.917 (8)	95487.503 ^b	2.468	95452.782 (13)	95450.915 ^a	1.867	95419.649 (11)	95417.545 ^b	2.104	95425.175 (20)	95385.285 ^a	2.051
15	95548.013 (-2)	95545.171 ^b	2.842	95509.424 (-19)	95507.244 ^a	2.180	95474.974 (4)	95472.625 ^b	2.349	95480.738 (-4)	95439.074 ^a	2.359
16	95609.965 (19)	95606.806 ^b	3.159	95569.761 (40)	95567.313 ^a	2.448	95533.979 (32)	95532.195 ^b	2.784	95539.959 (-6)	95496.438 ^a	2.651
17	95675.772 (14)	95672.162 ^b	3.609	95633.927 (15)	95631.120 ^a	2.807	95596.661 (-39)	95593.595 ^b	3.066	95602.894 (-2)	95557.375 ^a	2.980
18	95745.428 (-16)	95741.453 ^b	3.975	95701.809 (11)	95700.660 ^a	3.149	95663.019 (-6)	95659.505 ^b	3.514	95669.495 (-6)	95625.222 (-2)	3.339
19	95818.933 (-15)	95814.531 ^b	4.402	95773.538 (-20)	95773.055 (-41)	3.930	95733.055 (-11)	95729.125 ^b	3.924	95739.780 (-1)	95693.958 ^a	3.697
20	95896.283 (16)	95891.400 ^b	4.883	95848.955 (25)	95848.473 (-44)	4.368	95806.743 (-41)	95802.375 ^b	4.368	95813.762 (1)	95761.600 ^a	4.039
21	95977.503 (-5)	95972.079 ^b	5.424	95928.090 (90)	95928.090	4.668	95884.013 (15)	95879.345 ^b	4.668	95891.402 (-7)	95836.803 ^a	4.534
22	96062.534 (-24)			96011.085		5.304	95965.129 (-14)	95959.825 ^b	5.304	95973.720 (-6)	95915.565 ^a	4.946
23	96151.401 (-11)			96097.514			96049.800 (112)	96058.072 (1)		96058.072 (1)	95997.887 ^a	5.375
24	96244.129 (5)			96188.225			96137.973 (-8)	96146.373 (5)		96146.373 (5)	96083.760 ^a	
25	96340.657 (-31)			96282.196			96229.827 (1)	96238.694 (-23)		96238.694 (-23)	96173.183 ^a	
26	96440.956 (77)			96379.454			96326.848 (1)	96334.675 (-18)		96334.675 (-18)	96218.010 (-20)	
27	96544.934 (1)			96480.902				96537.662 (8)		96537.662 (8)	96312.703 (14)	
28	96652.787 (1)			96586.468				96644.586 (-16)		96644.586 (-16)	96410.928 (23)	
29	96764.482 (1)							96755.095 (63)		96755.095 (63)	96512.597 (-22)	
30	96879.924 (1)							96869.400		96869.400	96617.699 (1)	
31	96999.193 (1)							96987.277		96987.277	96726.316 (2)	
32	97121.216							97108.781		97108.781	96838.360 (0)	
33	97247.894							97233.816		97233.816	96953.966 (-73)	
34	97378.471							97357.920		97357.920	97072.814	
35	97512.670										97195.137	

Notes. ^(b) Data from Baker et al. (1993). ^(a) Data from Ubachs et al. (2000). ^(c) Data calculated from the e -parity levels. ^(d) Data calculated from the e -parity levels using the deperturbation described in Ubachs et al. (2000).

Table A.31. Molecular constants T_v , B_v , and D_v of the six CO isotopologues for each state, B^{Σ^+} , C^{Σ^+} , and E^{Π} for e^- and f^- parity (D_v is always kept as a free parameter in the fitting process).

	T_0		B_0		$-D_0$ ($\times 10^{-6}$)		T_v		B_v		$-D_v$ ($\times 10^{-6}$)		T_v		B_v		$-D_v$ ($\times 10^{-6}$)	
	T_v	B_v	$-D_v$ ($\times 10^{-6}$)	T_v	B_v	$-D_v$ ($\times 10^{-6}$)	T_v	B_v	$-D_v$ ($\times 10^{-6}$)	T_v	B_v	$-D_v$ ($\times 10^{-6}$)	T_v	B_v	$-D_v$ ($\times 10^{-6}$)	T_v	B_v	$-D_v$ ($\times 10^{-6}$)
1216	0.0000 (0)	1.92253 (0)	-6.121 (0)	91919.0328 (53)	1.94336 (2)	-6.363(16)	92929.9358 (40)	1.94090 (20)	-9.042(190)	92929.9317 (54)	1.95270 (4)	-6.454(62)	95082.8140 (227)	1.92879 (24)	-8.616(523)	95082.8140 (227)	1.92879 (24)	-8.616(523)
1217	0.0000 (0)	1.87396 (0)	-5.815 (0)	91918.9284 (85)	1.89464 (4)	-5.914(40)	92929.7231 (53)	1.89129 (24)	-7.715(522)	92929.6481 (53)	1.90387 (5)	-6.801(82)	95055.9701 (259)	1.88372 (40)	-13.559(1204)	95055.9701 (259)	1.88372 (40)	-13.559(1204)
1218	0.0000 (0)	1.83098 (0)	-5.551 (0)	91918.8543 (25)	1.85142 (1)	-5.641(8)	92929.5590 (44)	1.84697 (33)	-6.089(480)	92929.5452 (45)	1.85702 (4)	-5.871(55)	95031.9316 (228)	1.83783 (23)	-7.989(453)	95031.9316 (228)	1.83783 (23)	-7.989(453)
1316	0.0000 (0)	1.83797 (0)	-5.593 (0)	91919.0551 (37)	1.85845 (1)	-5.690(10)	92929.7536 (39)	1.85712 (121)	-9.292(1008)	92929.7481 (43)	1.86675 (5)	-5.676(84)	95035.9422 (127)	1.84490 (12)	-7.970(242)	95035.9422 (127)	1.84490 (12)	-7.970(242)
1317	0.0000 (0)	1.78940 (0)	-5.301 (0)	91918.8853 (80)	1.80969 (3)	-5.404(27)	92929.4750 (87)	1.80440 (24)	-4.433(413)	92929.4750 (87)	1.82811 (6)	-5.989(78)	95008.5805 (140)	1.79498 (10)	-5.009(136)	95008.5805 (140)	1.79498 (10)	-5.009(136)
1318	0.0000 (0)	1.74641 (0)	-5.049 (0)	91918.7947 (23)	1.76641 (1)	-5.130(5)	92929.2758 (76)	1.75965 (93)	-3.196(715)	92929.2758 (76)	1.78395 (3)	-5.516(22)	94983.9515 (176)	1.75065 (20)	-0.856(856)	94983.9515 (176)	1.75065 (20)	-0.856(856)
1216	88998.3150 (97)	1.92199 (5)	-7.408(41)	94065.5649 (47)	1.92385 (3)	-6.337(24)	95082.7605 (454)	1.90270 (5)	-9.413(114)	95082.7605 (454)	1.94090 (20)	-9.042(190)	97153.8983 (54)	1.89151 (6)	-9.328(113)	97153.8983 (54)	1.89151 (6)	-9.328(113)
1217	88972.9899 (174)	1.87334 (19)	-4.528(371)	94038.5061 (64)	1.87569 (8)	-5.761(162)	95055.9480 (237)	1.85644 (95)	-12.927(10413)	95055.9480 (237)	1.89129 (24)	-7.715(522)	97103.7201 (88)	1.84493 (36)	-6.806(930)	97103.7201 (88)	1.84493 (36)	-6.806(930)
1218	88950.2474 (34)	1.83120 (2)	-6.593(24)	94014.3118 (77)	1.83317 (6)	-5.644(88)	95032.0645 (469)	1.81424 (34)	-6.456(3105)	95032.0645 (469)	1.84697 (33)	-6.089(480)	97058.4630 (18)	1.80427 (6)	-9.835(410)	97058.4630 (18)	1.80427 (6)	-9.835(410)
1316	88954.0973 (40)	1.83818 (3)	-6.715(55)	94018.5116 (213)	1.83959 (9)	-5.051(72)	95035.6846 (2739)	1.82118 (9)	-8.275(237)	95035.6846 (2739)	1.85712 (121)	-9.292(1008)	97066.0601 (37)	1.81106 (4)	-8.390(90)	97066.0601 (37)	1.81106 (4)	-8.390(90)
1317	88928.1002 (139)	1.78966 (17)	-5.212(352)	93990.4543 (194)	1.79134 (12)	-4.405(130)	95008.6131 (296)	1.77361 (5)	-7.524(132)	95008.6131 (296)	1.80440 (24)	-4.433(413)	96967.8062 (26)	1.72321 (4)	-6.896(82)	96967.8062 (26)	1.72321 (4)	-6.896(82)
1318	88904.7410 (31)	1.74738 (2)	-5.975(27)	93965.8762 (64)	1.74951 (4)	-5.280(38)	94984.1816 (2353)	1.73261 (5)	-7.524(132)	94984.1816 (2353)	1.75965 (93)	-3.196(715)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1216	90988.2294 (126)	1.87355 (47)	9.682(3169)	96176.9248 (190)	1.90283 (19)	-5.197(343)	96076.3267 (238)	1.80991 (190)	32.499(*)	96076.3267 (238)	1.80991 (190)	32.499(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1217	90899.3726 (195)	1.78362 (155)	39.098(*)	96076.3267 (238)	1.80991 (190)	32.499(*)	96076.3267 (238)	1.80991 (190)	32.499(*)	96076.3267 (238)	1.80991 (190)	32.499(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1316	90906.3225 (105)	1.79341 (47)	12.410(3659)	96084.2280 (245)	1.81989 (92)	-1.736(*)	96084.2280 (245)	1.81989 (92)	-1.736(*)	96084.2280 (245)	1.81989 (92)	-1.736(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1317	90815.2393 (1206)	1.69520 (235)	37.719(8152)	95981.2762 (379)	1.72615 (143)	43.594(9531)	95981.2762 (379)	1.72615 (143)	43.594(9531)	95981.2762 (379)	1.72615 (143)	43.594(9531)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1216				98244.5110 (415)	1.87571 (72)	-1.933(*)	98244.5110 (415)	1.87571 (72)	-1.933(*)	98244.5110 (415)	1.87571 (72)	-1.933(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1217				98167.0437 (798)	1.82668 (813)	8.705(*)	98167.0437 (798)	1.82668 (813)	8.705(*)	98167.0437 (798)	1.82668 (813)	8.705(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1218				98097.5876 (428)	1.78947 (161)	9.638(*)	98097.5876 (428)	1.78947 (161)	9.638(*)	98097.5876 (428)	1.78947 (161)	9.638(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1316				98109.1420 (705)	1.79608 (198)	4.310(*)	98109.1420 (705)	1.79608 (198)	4.310(*)	98109.1420 (705)	1.79608 (198)	4.310(*)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)
1317				97958.4479 (263)	1.71070 (65)	-8.017(2855)	97958.4479 (263)	1.71070 (65)	-8.017(2855)	97958.4479 (263)	1.71070 (65)	-8.017(2855)	98735.1064 (170)	1.61846 (60)	-38.301(3880)	98735.1064 (170)	1.61846 (60)	-38.301(3880)

Notes. Standard errors are given in parentheses in units of the least significant digit, and for D_v , an asterisk indicates that the standard error is higher than 50% of the value. A ninth-order polynomial is used for the ground state X0.

Table A.32. Molecular constants $T_v(1)$, q_v , and q_{Dv} of the six CO isotopologues for the $E^1\Pi$ state, calculated from the previous table: $T_v(J=1)$ is the average of T_v for e - and f -parity, $q_v = B_e - B_f$, and $q_{Dv} = D_e - D_f$.

Species	$T_v(1)$	q_v	$q_{Dv} (\times 10^{-6})$
E00			
1216	92929.9338(47)	0.01186(3)	-0.06(4)
1217	92929.6856(53)	0.01092(5)	0.50(10)
1218	92929.5521(44)	0.01080(4)	-0.12(6)
1316	92929.7509(41)	0.01093(3)	-0.24(5)
1317	92929.4750(87)		
1318	92929.3180(66)	0.01043(4)	-1.27(6)
E10			
1216	95082.7873(341)	0.01211(22)	-0.43(36)
1217	95055.9591(248)	0.00757(32)	5.84(86)
1218	95031.9981(348)	0.00914(28)	1.90(47)
1316	95035.8134(1433)	0.01222(67)	-1.32(63)
1317	95008.5968(218)	0.00942(17)	0.58(27)
1318	94984.0666(1264)	0.00900(57)	-2.34(79)
E20			
1216	97153.8909(51)	0.01119(6)	-0.09(11)
1217	97103.6839(125)	0.01151(65)	-6.12(617)
1218	97058.4695(44)	0.00997(20)	3.38(176)
1316	97066.0606(47)	0.01012(6)	0.12(16)
1317			
1318	96967.8012(29)	0.00940(4)	-0.63(11)
E30			
1216	98919.6966(210)	0.00865(30)	3.04(78)
1217	98873.3328(243)	0.00842(177)	14.65(2376)
1218	98829.3377(197)	0.00894(75)	-0.93(537)
1316	98836.9001(338)	0.01193(156)	-26.64(1323)
1317			
1318	98735.1112(120)	0.00832(42)	3.01(275)

Notes. The standard errors, in parentheses, are expressed in units of the least significant digit.

Table A.33. Molecular constants q_v and q_{Dv} of the six CO isotopologues for the $E^1\Pi$ state, obtained from a second-order regression through the data.

Species	N	q_v	$q_{Dv} (\times 10^{-6})$
E00			
1216	29	0.01173(9)	0.10(12)
1217	26	0.01082(21)	0.61(31)
1218	26	0.01084(10)	-0.27(15)
1316	25	0.01107(19)	-0.54(32)
1317			
1318	26	0.01112(35)	-2.41(53)
E10			
1216	21	0.01133(29)	0.55(67)
1217	18	0.00848(60)	2.75(183)
1218	22	0.01025(37)	0.23(76)
1316	22	0.01140(208)	-1.13(434)
1317	22	0.00996(15)	-0.21(32)
1318	22	0.00943(36)	0.13(74)
E20			
1216	23	0.01108(20)	0.09(38)
1217	12	0.01128(185)	-4.08(1198)
1218	14	0.00967(67)	0.33(328)
1316	21	0.00998(14)	0.51(25)
1317			
1318	21	0.00947(10)	-0.80(23)
E30			
1216	22	0.00832(38)	4.11(79)
1217	8	0.00842(183)	14.69(2463)
1218	11	0.00958(104)	-6.38(793)
1316	13	0.00792(96)	5.96(279)
1317			
1318	12	0.00832(76)	3.05(494)

Notes. The standard errors, in parentheses, are expressed in units of the least significant digit. N is the number of data.

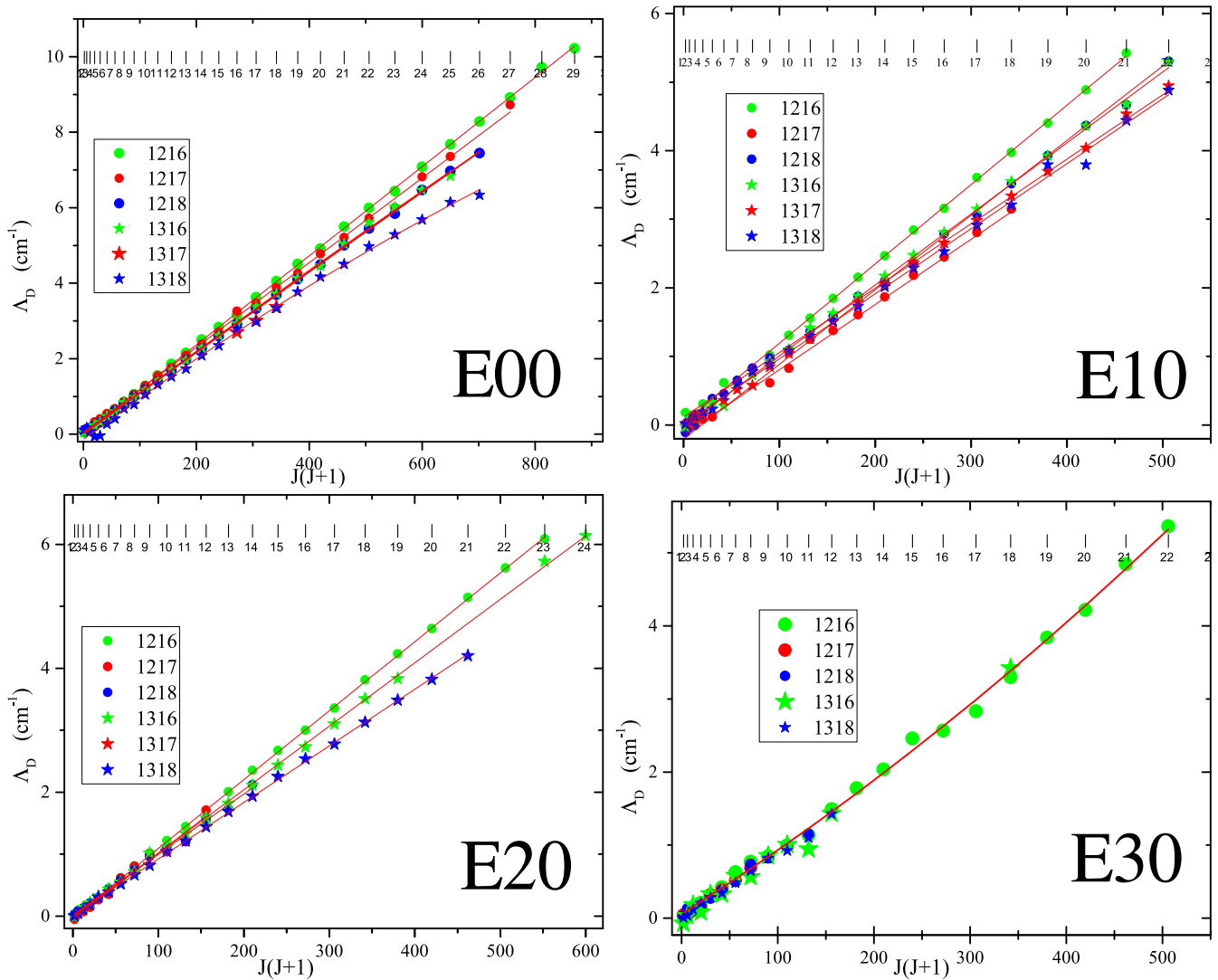


Fig. A.37. Λ -type doubling (in cm^{-1}) vs. $J \times (J + 1)$ of E00, E10, and E20 for the six isotopologues and of E30 for five isotopologues. For E10, we combined our dataset for the R - and P -branches and the Q -branch of Ubachs et al. (2000). A polynomial fit is also drawn; it is linear in most cases.

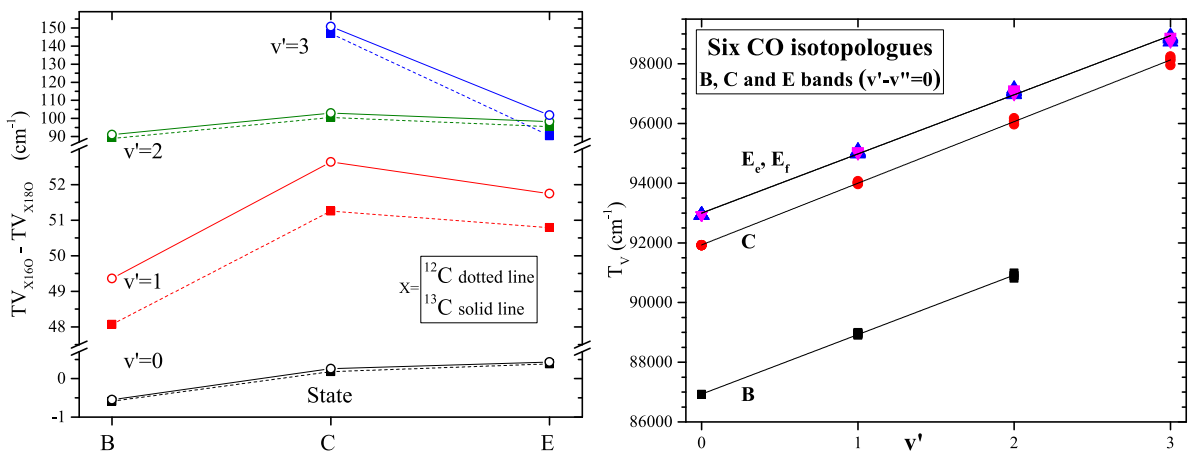


Fig. A.38. Trend comparison for the six CO isotopologues. *Left:* term value differences between ^{16}O - and ^{18}O -bearing isotopologues for ^{12}C and ^{13}C (dotted and solid lines, respectively) versus the B , C , and E states. *Right:* T_v versus v' for the B , C , and E states (each datapoint contains up to six isotopologues). For each state, a linear fit is drawn through all isotopologues.

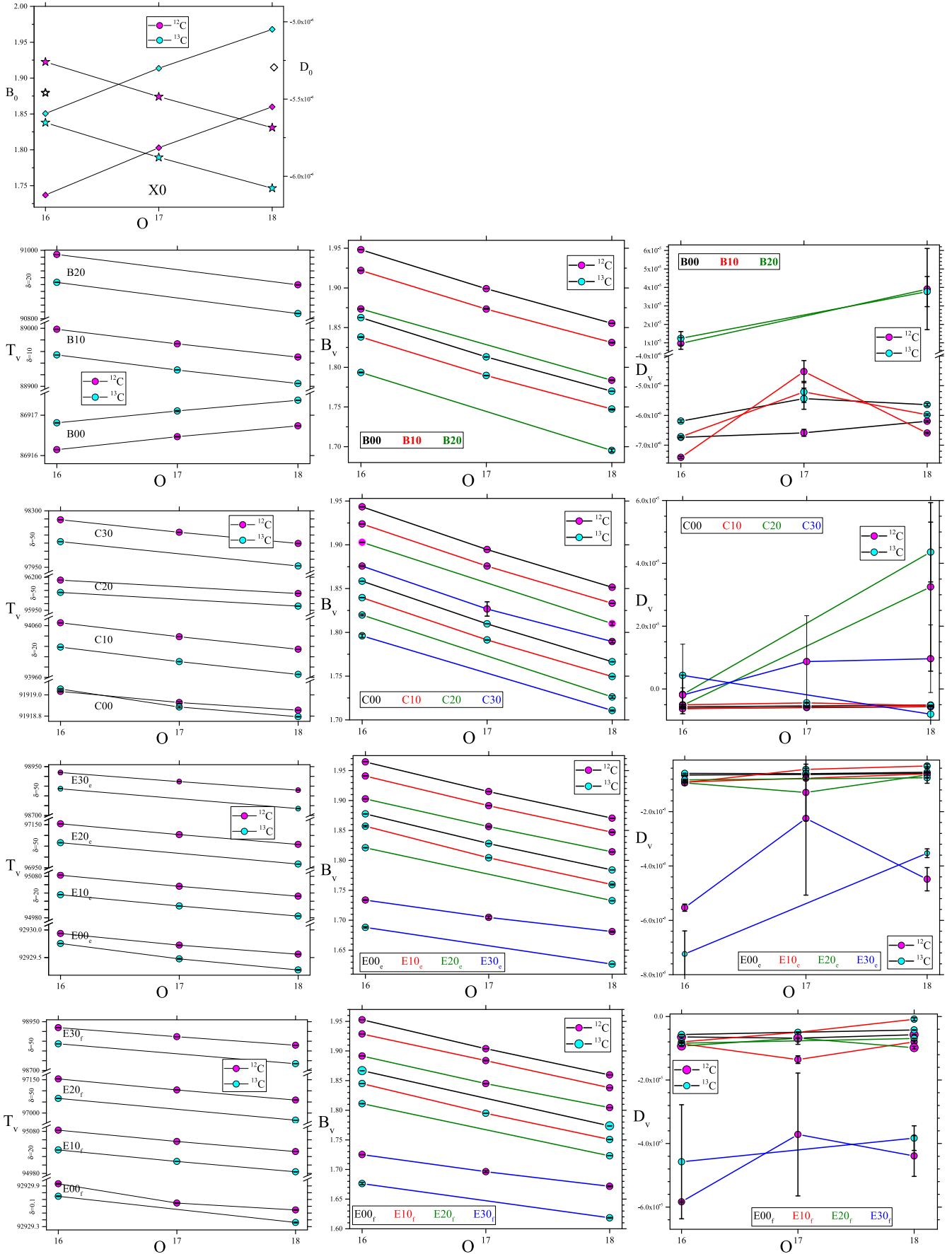


Fig. A.39. Molecular constants for the six CO isotopologues. *Top row:* B_0 and D_0 for $v''=0$ of the $X^1\Sigma^+$ ground state ($T_0=0$ for all). The standard deviation (at 2σ) is shown between two short horizontal bars. For T_V , all values are in cm^{-1} , with δ values indicating the local spacing between ticks.