

ACCURATE LABORATORY WAVELENGTHS OF THE VACUUM ULTRAVIOLET $A(v' = 3)$ – $X(v'' = 0)$ BAND OF $^{12}\text{C}^{17}\text{O}$ AND $^{12}\text{C}^{18}\text{O}$

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ABSTRACT

Six individual rotational lines ($J'' \leq 3$) of $^{12}\text{C}^{17}\text{O}$, as well as four of $^{12}\text{C}^{18}\text{O}$, were detected in the $A^1\Pi(v' = 3)$ – $X^1\Sigma^+(v'' = 0)$ vibronic band, and their wavelengths determined using neighboring $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ lines as reference. The measurements (fluorescence excitation spectra) were performed in a pulsed supersonic jet (Ar or Ne as carrier gas) employing a tunable pulsed vacuum ultraviolet radiation source with a narrow bandwidth (~ 5 GHz). The new spectral data on $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ are applied to the interpretation of recent vacuum ultraviolet observations of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ in the interstellar medium.

Subject headings: ISM: molecules — methods: laboratory — molecular data — ultraviolet: general

1. INTRODUCTION

Carbon monoxide (CO) is one of the most extensively studied molecules both in the laboratory and in astrophysical observations. The relevance of CO in astrophysics results from its high abundance in interstellar clouds (van Dishoeck & Black 1988) and from its well-observable spectra in the vacuum ultraviolet and infrared as well as in the millimeter-wave regions. Detection and quantification of the different stable isotopomers of CO in the interstellar medium are of particular interest for the modeling of interstellar clouds and stellar evolution (Balsler, McMullin, & Wilson 2002).

The electronic transitions of CO isotopomers in the interstellar medium are detected as absorption lines in the vacuum ultraviolet radiation from suitable stellar sources. Rotationally resolved vacuum ultraviolet spectra of interstellar CO, consisting of vibronic bands of the fourth-positive $A^1\Pi$ – $X^1\Sigma^+$ band system, have been measured for $^{12}\text{C}^{16}\text{O}$ (Smith et al. 1991), $^{13}\text{C}^{16}\text{O}$ (Sheffer et al. 1992), $^{12}\text{C}^{18}\text{O}$, and $^{12}\text{C}^{17}\text{O}$ (Sheffer, Lambert, & Federman 2002). Due to the low temperature in the interstellar medium, only transitions from the lowest rotational states of the $A(v' = i)$ – $X(v'' = 0)$ band system with $J'' \leq 2$ are observed (Morton & Noreau 1994). These results are employed to determine the column densities and isotopic ratios of CO, the temperature and heliocentric velocity of the gas, the associated density of molecular hydrogen, as well as structural details of the interstellar gas clouds (Smith et al. 1991).

For a proper interpretation of the ultraviolet absorption spectra of interstellar CO isotopomers, accurate rest wavelengths from rotationally resolved laboratory spectra are needed. Wavelength data for all astrophysically relevant $A(v' = i)$ – $X(v'' = 0)$ vibronic bands of $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ have been compiled by Morton & Noreau (1994). Beaty, Braun, & Huber (1997) published the spectroscopic data for $v' = 0$ –9 of $^{12}\text{C}^{18}\text{O}$. However, when Sheffer et al. (2002) recently reported the first detection of interstellar $^{12}\text{C}^{17}\text{O}$, no laboratory wavelengths were available for the $v' = 2$ –5 bands of $^{12}\text{C}^{17}\text{O}$. Sheffer et al. used rest wavelengths for $^{12}\text{C}^{17}\text{O}$ that were calculated from the Dunham coefficients of $^{12}\text{C}^{16}\text{O}$ by appropriate isotopic corrections. The use of these calculated rest wavelengths for $^{12}\text{C}^{17}\text{O}$ resulted in an apparent

difference between the heliocentric velocity obtained from the $^{12}\text{C}^{17}\text{O}$ data and that obtained from the $^{12}\text{C}^{18}\text{O}$ data measured in the same interstellar cloud region, which raised concerns about the accuracy of these calculated wavelengths.

In this Letter, we report laboratory-measured vacuum ultraviolet transition wavelengths of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$, obtained by selectively exciting single rovibronic transitions in the $A(v' = 3)$ – $X(v'' = 0)$ band of the molecule by narrow bandwidth vacuum ultraviolet radiation and detecting the resulting fluorescence. The laser-induced fluorescence excitation spectra were measured in a natural CO gas sample flow-cooled in a supersonic jet. Each spectrum covered the bands of $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, as well as $^{12}\text{C}^{17}\text{O}$. This allowed an accurate calibration of the wavelengths of the $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$ lines using the lines of the more abundant isotopomers as standards.

2. EXPERIMENTAL METHOD

The experimental setup is illustrated schematically in Figure 1. A wavelength-tunable pulsed light source ($\tau \sim 25$ ns) is used that emits narrow bandwidth ($\Delta\nu \sim 5$ GHz) vacuum ultraviolet radiation in the 1430–1470 Å region. The vacuum ultraviolet radiation is generated by two-photon resonant four-wave sum frequency mixing (Yamanouchi & Tsuchiya 1995) of two pulsed dye laser beams in a magnesium vapor-krypton gas mixture, prepared inside a heat pipe oven system as described by Scheingraber & Vidal (1981). The two dye lasers (both Lambda Physik, FL 3001X with Coumarin 440 dye) are pumped by the same XeCl excimer laser (Lambda Physik, EMG 203 MSC). The heat pipe system is equipped with an MgF₂ window at the beam exit side and is directly attached to the vacuum system.

The sample of CO gas, containing the isotopomers of CO in natural abundance, is seeded into a pulsed free supersonic jet. Adequate cooling is obtained with up to 25% CO gas in either argon or neon as carrier gas. This gas mixture is allowed to expand from a stagnation pressure of 3–4 bars through an orifice 0.8 mm in diameter into the vacuum chamber kept at circa 5×10^{-6} mbar by a turbo molecular pump (Pfeiffer, model TPH200). A delay generator (Stanford Research Systems, model DG 535) is used for synchronization of the lasers with the pulsed gas valve (General Valves, series 9, pulse duration ~ 2 ms). The vacuum ultraviolet beam crosses the supersonic jet perpendicularly about 25 nozzle diameters downstream from the nozzle.

The undispersed fluorescence from the irradiated volume in

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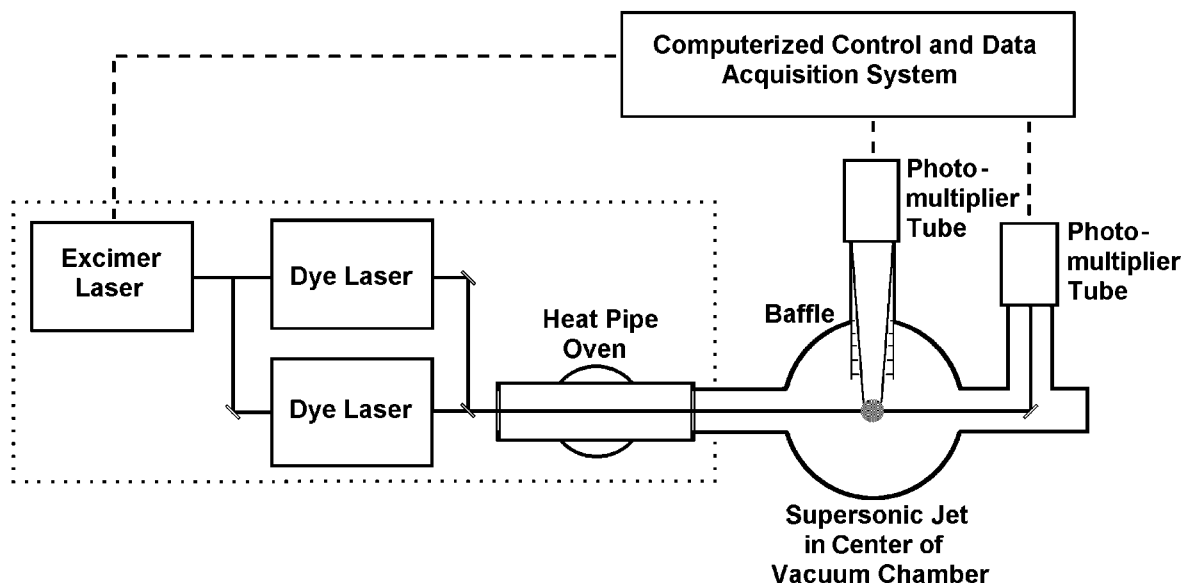


FIG. 1.—Schematic illustration of the experimental setup for vacuum ultraviolet laser-induced fluorescence excitation spectroscopy of a flow-cooled sample. The dotted line indicates the part of the setup constituting the tunable narrow bandwidth vacuum ultraviolet source. The dashed lines indicate connections with the control and data acquisition system.

the jet is measured by a solar blind photomultiplier tube (EMR Photoelectric, model 542G-08-18-03900) positioned perpendicular to both the laser beams and the jet. Noise from scattered light is reduced to a level lower than the detection limit by a baffle in front of the photomultiplier. A second photomultiplier tube (Hamamatsu, model R973) is used to measure the transmitted vacuum ultraviolet beam. The data acquisition system consists of two boxcar integrators (Stanford Research Systems, model SR250) and a computer interface (Stanford Research Systems, model SR245). A laser-induced fluorescence excitation spectrum is obtained by recording the fluorescence while scanning the vacuum ultraviolet excitation wavelength by tuning the wavelength of one dye laser. The experiment is controlled by a custom HP VEE (version 3.12) programme running on a personal computer.

3. RESULTS AND DISCUSSION

Six individual rotational lines of the $^{12}\text{C}^{17}\text{O}$ $A(v' = 3) - X(v'' = 0)$ vibronic band were detected (see Fig. 2) as well as

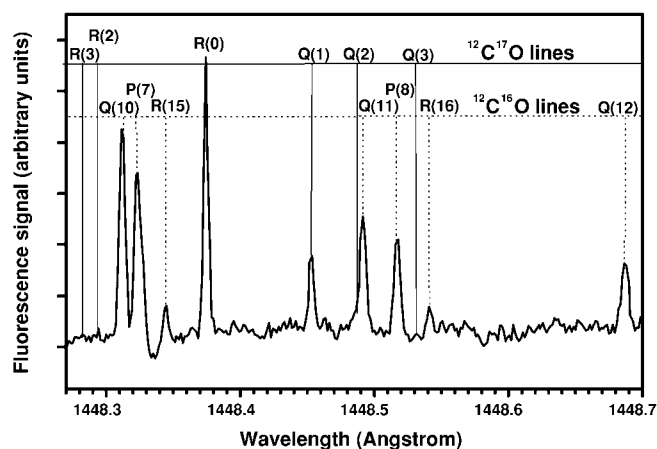


FIG. 2.—Typical fluorescence excitation spectrum showing the observable transitions of $^{12}\text{C}^{17}\text{O}$ (solid lines) among $^{12}\text{C}^{16}\text{O}$ transitions (dotted lines).

four lines of the $^{12}\text{C}^{18}\text{O}$ band. The numerical results are summarized in Table 1. In general, it was possible to detect the $Q(J'')$ and $R(J'')$ transitions originating from rotational levels with $J'' \leq 3$. From the line intensity ratios of the lowest rotational lines, the rotational temperature was estimated to be 4 ± 1 K, corresponding roughly to the temperatures in diffuse interstellar clouds (Morton & Noreau 1994). Note that this temperature is no more than a rough indication of the conditions in the jet.

The data of four different spectra similar to that of Figure 2, each containing the observable lines of both $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$, were combined to obtain the experimental wavelength data in Table 1. The wavelength scales of the experimental spectra were calibrated using the wavelengths of the $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ lines as published by Morton & Noreau (1994) and Tilford & Simmons (1972). When the wavelengths of the $A(v' = 3) - X(v'' = 0)$ band of $^{12}\text{C}^{16}\text{O}$ of Tilford & Simmons are compared with those of Morton & Noreau, the wavelengths of Tilford & Simmons appear to be shifted by 4.5×10^{-3} Å on average. For our calibration, the wavelengths of Morton & Noreau have been used as reference as far as possible. For the higher rotational lines of $^{12}\text{C}^{16}\text{O}$, the wavelengths of Tilford & Simmons were used after a correction for the apparent shift. The bandwidth of the vacuum ultraviolet radiation is the physical factor determining the precision of the measured wavelengths. The indicated errors in the wavelength positions of the lines are the average standard deviation of the least-squares calibration fits on the spectra, except for the weakest lines where larger errors were estimated. The hyperfine splitting of $^{12}\text{C}^{17}\text{O}$ is not observed since it is smaller than the experimental line widths of the rovibronic transitions (Lovas & Krupenie 1974).

The conditions in the supersonic jet were optimized to obtain extensive flow cooling of the sample. The low rotational temperature of the CO sample facilitates the measurement of the weak $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ spectral lines by reducing the intensities of the neighboring hot $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ lines that tend to obscure the weaker lines and by increasing the line intensity of the lower rotational lines ($J'' \leq 2$) of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$. The

TABLE 1
EXPERIMENTAL $^{12}\text{C}^{17}\text{O}$ AND $^{12}\text{C}^{18}\text{O}$ WAVELENGTH DATA COMPARED WITH DATA USED BY SHEFFER ET AL. 2002 AS WELL AS RESULTING HELIOCENTRIC VELOCITIES TOWARD X PERSEI

A–X(3–0) Line	SHEFFER ET AL.	DATA OBTAINED IN PRESENT EXPERIMENT		
	λ_0 (Å)	λ_0 (Å)	Signal-to-Noise Ratio	Line Width (mÅ)
$^{12}\text{C}^{18}\text{O}$				
<i>R</i> (1)	1449.248 ^a	$(1449.249 \pm 2) \times 10^{-3}$	20	...
<i>R</i> (0)	1449.294 ^a	$(1449.295 \pm 2) \times 10^{-3}$	60	4.2
<i>Q</i> (1)	1449.371 ^a	$(1449.373 \pm 2) \times 10^{-3}$	19	4.2
<i>Q</i> (2)	$(1449.404 \pm 2) \times 10^{-3}$	3	6
v_{helio} (km s ⁻¹) ^b	15.0	14.7 ± 0.4		
$^{12}\text{C}^{17}\text{O}$				
<i>R</i> (3)	$(1448.283 \pm 4) \times 10^{-3}$	~1	...
<i>R</i> (2)	$(1448.297 \pm 4) \times 10^{-3}$	~1	...
<i>R</i> (1)	1448.332 ^c
<i>R</i> (0)	1448.379 ^c	$(1448.375 \pm 2) \times 10^{-3}$	20	5
<i>Q</i> (1)	1448.458 ^c	$(1448.453 \pm 2) \times 10^{-3}$	7	5
<i>Q</i> (2)	$(1448.484 \pm 4) \times 10^{-3}$	~1	...
<i>Q</i> (3)	$(1448.532 \pm 4) \times 10^{-3}$	~1	...
v_{helio} (km s ⁻¹) ^b	13.5	14.4 ± 0.4		

NOTE.—The *R*(1) line of $^{12}\text{C}^{17}\text{O}$ and the *R*(2) line of $^{12}\text{C}^{18}\text{O}$ were not detected because of overlap with the stronger *P*(7) line of $^{12}\text{C}^{16}\text{O}$ and the *Q*(1) line of $^{13}\text{C}^{16}\text{O}$, respectively.

^a The wavelengths were calculated by Sheffer et al. 2002 from the term values of Beatty et al. 1997.

^b The heliocentric velocities of the interstellar CO toward X Persei were calculated by using the corresponding λ_0 -values.

^c The wavelengths calculated by Sheffer et al. 2002 from $^{12}\text{C}^{16}\text{O}$ data by correcting for the isotopic shift.

fact that the low rotational temperature reduces the number of transitions of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ that can be detected to those originating from low rotational levels with $J'' \lesssim 3$ is not considered a disadvantage since these are also the only transitions observable in the interstellar medium.

The new spectral data reported here can be applied to address the problem previously encountered with the interpretation of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ absorption spectra measured in interstellar clouds, as reported by Sheffer et al. (2002). Under the conditions of our experiment, our laser-induced fluorescence excitation spectrum can be shown to be essentially equivalent to an absorption spectrum with extremely high sensitivity (Demtröder 1996). In Table 1, our data are compared with the rest wavelengths used by Sheffer et al. (2002) for the *A*($v' = 3$)–*X*($v'' = 0$) band. Sheffer et al. reported a discrepancy of 1.5 km s⁻¹ in the heliocentric velocities (v_{helio}) calculated for the interstellar CO when using the rest wavelengths of $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$ that they had at their disposal. It is, however, physically improbable to observe different Doppler shifts for the two isotopomer spectra measured in the same sample space under the same conditions. Using our experimental rest wavelengths, the difference in the heliocentric velocity is reduced to 0.3 km s⁻¹, which is smaller than the error of 0.4 km s⁻¹ on the values. As anticipated by Sheffer et al. (2002), the correction of a systematic shift in the $^{12}\text{C}^{17}\text{O}$ rest wavelengths contributed most to equalize the calculated heliocentric velocities.

4. CONCLUDING REMARKS

The combination of a tunable narrow bandwidth vacuum ultraviolet laser source and an optimized experimental setup for measuring the laser-induced fluorescence excitation spectra

of a flow-cooled sample in a supersonic jet facilitated the measurement of the $J'' \leq 3$ rotational lines of the *A*($v' = 3$)–*X*($v'' = 0$) vibronic band of $^{12}\text{C}^{17}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ in natural abundance. The narrow bandwidth of the vacuum ultraviolet source yielding high-resolution spectra, the high sensitivity of the laser-induced fluorescence method, and the simplification of the spectra due to cooling of the rotational degrees of freedom in the supersonic jet made these measurements possible. We found that the use of our experimental wavelength data solves the interpretation problem encountered by Sheffer et al. (2002) regarding the calculation of heliocentric velocities within the accuracy limits of our measurements.

The spectral results on $^{12}\text{C}^{17}\text{O}$ are to our knowledge the first rotationally resolved laboratory measurements reported on the *A*–*X* band system of this isotopomer. There is a need for more extensive laboratory measurements to characterize the *A*–*X* bands of $^{12}\text{C}^{17}\text{O}$ that are of astrophysical interest (Morton & Noreau 1994; Sheffer et al. 2002). The laser spectroscopy on flow-cooled CO isotopomers will be continued in our laboratory and extended to other vibronic bands of the *A*–*X* system.

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