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Theoretical and revisited experimentally retrieved He-broadened line parameters of carbon monoxide in the fundamental band

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ABSTRACT

We report revisited experimentally retrieved and theoretically calculated He-broadened Lorentz half-width coefficients and He- pressure-shift coefficients of 45 carbon monoxide transitions in the 1←0 band. The spectra analyzed in this study were recorded over a range of temperatures between 79 and 296 K. The He-broadened line parameters and their temperature dependences were retrieved using a multispectrum nonlinear least squares analysis program. The line shape models used in this study include Voigt, speed dependent Voigt, Rautian (to take into account confinement narrowing) and Rautian with speed dependence, all with an asymmetric component added to account for weak line mixing effects. We were unable to retrieve the temperature dependence of line mixing coefficients. A classical method was used to determine the He-narrowing parameters while quantum dynamical calculations were performed to determine He-broadening and He-pressure shifts coefficients at different temperatures. The line mixing coefficients were also derived from the exponential power gap law and the energy corrected sudden approximation. The current measurements and theoretical results are compared with other published results, where appropriate.

1. Introduction

Carbon monoxide is present as a trace constituent in the Earth and planetary atmospheres, as well as in the interstellar medium (see for example, [1–4] and references therein). For decades, spectral line shape studies of self- and foreign-broadened ro-vibrational lines of CO have captivated the interest of experimentalists and theoreticians (e.g. [5–24]). Many of these spectroscopic studies have been triggered by the need for highly accurate line parameters for the interpretation of atmospheric spectra recorded by spectroscopic remote sensing instruments on ground, balloon or satellite platforms. A literature review of studies of the CO–He molecular system is given below.

One of the earlier line shape studies of carbon monoxide transitions was by Nerf and Sonnenberg [12] who

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investigated the carbon monoxide R(0) line located at 115 GHz. The authors measured the pressure broadening coefficients of CO broadened by hydrogen, deuterium, helium, neon, and argon for the $J=1\leftarrow 0$ transition at three different temperatures (77 K, 195 K and 294 K). Monnanteuil and Colmont [13] measured the foreign (N_2, O_2, and He) and self-broadening coefficients of carbon monoxide transitions in the millimeter range ($\sim$230 GHz) for temperatures in the 220 to 300 K range.

Boissoles et al. [14] have reported the theoretical line mixing coefficients of CO perturbed by He employing the infinite order sudden approximation (IOSA) and the energy corrected sudden approximation (ECSA) techniques. Green et al. [15] have computed the theoretical off-diagonal collision induced broadening cross sections for the $1\leftarrow 0$ band of CO broadened by helium. The authors have compared experimental spectra of CO broadened by He recorded at temperatures of 78–292 K with spectra calculated line-by-line with contributions from theoretical line mixing. The helium and hydrogen broadened pressure - shift coefficients in carbon monoxide absorption spectra have been measured by Mannucci [16] for three ro-vibrational lines, P(8), R(2), and R(14), of the fundamental band in the infrared region. An infrared heterodyne spectrometer with a spectral resolution of 20 MHz was used in this study.

The line mixing parameters and pressure-induced shift coefficients from room-temperature CO spectra broadened by He in the $1\leftarrow 0$ and $2\leftarrow 0$ bands have been measured and calculated by Thibault et al. [17]. Pressure broadening coefficients were also measured at room temperature and at 85 K in the $1\leftarrow 0$ band in the latter study. The authors compared their experimental results with theoretical values [15] obtained from quantum dynamical calculations. Duggan et al. [18] have studied the high resolution (10^{-4} cm^{-1}) infrared spectra of carbon monoxide diluted by Xe, N_2, and He in the intermediate pressure range. The high signal-to-noise ratio of the spectra ($\sim$2000:1) allowed the authors to quantify the speed dependent collisional broadening effects on the retrieved line parameters. A Fourier transform spectrometer was used by Bouanich et al. [19] to record the absorption spectra of CO diluted by He, Ne, Ar, Xe, O_2, and N_2 in the $1\leftarrow 0$ band. The authors compared their experimental pressure-shift coefficients with the theoretical computations using a semi-classical model.

Henry et al. [20] used a tunable diode laser spectrometer system attached to a Michelson interferometer to measure the R(21), R(23) and R(24) transitions of the fundamental band of CO perturbed by He, Ne, Xe and N_2 at pressures between 10 and 600 Torr. The authors have retrieved the broadening, narrowing and pressure induced shift parameters using several line shape models such as the Voigt, Galatry (i.e. soft collision model) and Rautian (i.e. hard collision model). They also analyzed those spectra and compared the results with two new semi-empirical models generated by the convolution of Lorentzian with soft and hard collision models.

Beaky et al. [21] have measured the pressure broadening and shift parameters for the R(0) and R(1) pure rotational transitions of CO broadened by helium for temperatures between 1 and 600 K using the collisional cooling technique. Simultaneous close-coupling (CC) calculations of these parameters performed by Thachuk et al. [22] on different potential energy surfaces (PES) were shown to lead to good agreement with the measured values down to about 12 K. Below an important mismatch between calculated and measured values is observed even using the best PES.

Sinclair et al. [23] published the CO–He broadening coefficients for 39 lines in the P and R branches of the fundamental band using a difference frequency laser spectrometer with spectral resolution of 2 MHz. This experimental setup allowed them to record spectra with signal-to-noise ratio of 3000:1 at 301.5 K using a temperature stabilized gas absorption cell. The authors investigated the absorption spectra using the soft collision model. The room temperature broadening and shift parameters of CO broadened by He and Ar were measured by Luo et al. [24] for several R- and P- branch transitions in the same band. The difference frequency laser spectrometer used in their study was a modified, 3-channel version of the spectrometer described in Ref. [23]. An overall good agreement was observed between the measured results and close coupling dynamical calculations performed on the best available interaction potential.

The McMath-Pierce Fourier transform spectrometer facility located at the National Solar Observatory on Kitt Peak was used by Mantz et al. [25] to record the spectra of CO perturbed by helium. In this study, the authors have investigated the Lorentz pressure-broadening and pressure-induced shift coefficients along with their temperature dependences of P and R branch lines in the 2010 to 2260 cm^{-1} region for a temperature range between 80 and 297 K. The spectra were analyzed simultaneously using a multispectrum nonlinear least squares fitting technique [26].

Studies of helium broadened spectra of less-abundant isotopologues of carbon monoxide gas have also been carried out. For example, a Fourier transform spectrometer system composed of a tunable diode laser (TDL) coupled with a Michelson interferometer was employed by Mantz et al. [27] to measure the spectra of ^{13}CO broadened by helium over a wide range of temperatures from 11.5 to 298.6 K. For the P(2) line of the fundamental, the authors determined the He-broadened half width coefficient and its temperature dependence. Henry et al. [28] have reported the ^{13}CO–He broadening parameters taking confinement narrowing into account while fitting with the soft collision profile.

Thibault et al. [29] have reported the helium broadening coefficients of the R(0) and P(2) transitions of the fundamental band of ^{13}CO recorded at low temperatures (from 12 K up to room temperature) using a frequency stabilized diode laser system controlled by Michelson interferometer. The authors have determined the broadening coefficients by taking the narrowing effect into account using the Galatry profile. The fits using the soft collision model reproduced the experimental data better than the Voigt profile. The overall good agreement between measured pressure broadening and close coupling (CC) cross sections was observed to improve at temperatures below 30 K.