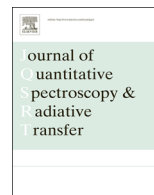




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## Spectral shape parameters of pure CO<sub>2</sub> transitions near 1.6 μm by tunable diode laser spectroscopy



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### ABSTRACT

Room temperature spectra of four lines of pure CO<sub>2</sub> in the 1.6 μm region have been measured in a wide range of pressure using a tunable diode laser spectrometer. The spectra of each line have been adjusted using a multi-spectrum fitting procedure with various line-shape models, including the recently recommended Hartmann-Tran profile (HTP). The results show that the collision-induced velocity changes and the speed-dependence effects are clearly observed. It is also shown that taking into account the correlation between velocity- and internal state-changes is necessary to obtain physically-meaningful line-shape parameters. The latter are reported and discussed.

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### 1. Introduction

With the tremendous advances in spectroscopy instrumentation, the use of the Voigt profile to describe the observed line shape is becoming obsolete. Various refined effects neglected by this profile, such as the collision-induced velocity changes (also called Dicke narrowing or collisional narrowing), the speed dependences of the collisional line width and shift, and the correlation between velocity and internal-state changes, must be taken into account. Recently, the partially-Correlated quadratic-Speed-Dependent Hard-Collision profile (also called the partially-Correlated quadratic-Speed-Dependent Nelkin-Ghatak or the Hartmann-Tran profile) was proposed to be a new standard for spectroscopic databases and radiative transfer calculations [1–3]. This profile takes into account all the above-mentioned effects. Furthermore, it can be quickly and easily computed numerically through some

combinations of the complex Voigt function [1,2]. The functional forms and algorithms for the calculation of this profile and its different limiting cases were provided [4,5]. Because of the importance of CO<sub>2</sub> for atmospheric applications, non-Voigt effects in CO<sub>2</sub> line shapes have been investigated for years (e.g. [6–17]). In most of the studies, the non-Voigt behavior of the line shape was assumed to be entirely due either to the Dicke narrowing effect [6,7,11,12,14,15] or to the speed dependences of the line width and shift [8–10,12,17] alone; only a few investigations have considered both effects simultaneously. In Ref. [13], thanks to high quality spectra and to the use of a multi-spectrum fitting technique, collisional narrowing and speed-dependence effects were observed for an air-broadened transition of CO<sub>2</sub> near 1.6 μm. The authors showed that both effects were necessary to describe the measured line shapes and to reduce the fit residuals down to the measurement-noise level. More recently, Bui et al. [16] extended this observation to two other lines of CO<sub>2</sub> in air in the 2.06 μm region. In addition to Dicke narrowing and speed-dependence effects, it was shown that the correlation between velocity- and state-changing collisions

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also contributes to the line shape. The authors then concluded that the most appropriate profile for the modeling of the line shapes of CO<sub>2</sub> in air in this spectral region is the partially-Correlated Speed-Dependent Nelkin–Ghatak profile.

In this work, the Hartmann-Tran profile (HTP) is used to analyze room temperature spectra of four lines of pure CO<sub>2</sub> in the 1.6 μm spectral region, measured in a wide range of pressure using a tunable diode laser spectrometer. Analyses are also carried using the usual Voigt profile and other simplified models taking into account either the Dicke narrowing or the speed-dependence effect.

## 2. Experimental details and data analysis

The spectra presented in this study have been measured using an external-cavity diode laser (ECDL) operating in the 6100–6400 cm<sup>-1</sup> spectral range (TOPTICA DL100prodesign, 1 MHz emission band width) and a White-type multi-pass absorption cell. This experimental set-up has been presented in a previous study devoted to pure CO<sub>2</sub> [18] where more details can be found. The signal-to-noise (S/N) ratio of our measured spectra is about 1000. Four lines have been retained for their line-shape analysis: the R(10), R(12) and R(20) lines of the (30013)←(00001) band and the P(38) line of the (30012)←(00001) band. These transitions allow to test the different line-shape models for a quite large range of the rotational quantum number *J*. Measurements were performed at room temperature (between 296 K and 297 K) and for a broad range of pressure (from 0.013 to 0.59 atm). All the considered lines are well isolated for the considered pressures. The optical path used varied from 8 to 32 m, depending on the line and on the pressure of the measurement. Table 1 gives a list of the considered lines as well as the pressure and optical path for each measurement. The corresponding Lorentz-to-Doppler widths ratio ( $\Gamma_L/\Gamma_D$ ) ranges are also reported.

As can be observed in Table 1, the considered pressure conditions lead to a large range of values for the  $\Gamma_L/\Gamma_D$  ratio, from the nearly purely Doppler regime (small value of  $\Gamma_L/\Gamma_D$ ) to collision-prevailing conditions (large value of  $\Gamma_L/\Gamma_D$ ). This will allow us to detect both the Dicke narrowing and the speed-dependence effects on the line shape. For this, a multi-spectrum fitting procedure, in which spectra measured at various pressures are simultaneously adjusted, has been used together with a variety of

line profiles. The simplest one considered here is the usual Voigt profile (VP) [20], which is a convolution of a Gaussian and a Lorentzian profiles. The second one is the Rautian (or Nelkin–Ghatak) profile which takes into account the effects of collision-induced velocity changes through the hard-collision limit (HC) [21,22]. The next profile is the Speed-Dependent Voigt profile (SDVP) [23] which generalizes the VP by including the speed dependences of the collisional width and shift. Both the Dicke narrowing and the speed-dependence usually induce a narrowing of the line but generally not in the same pressure regime so that a multi-spectrum fitting for a wide range of pressure should enable to distinguish between the two effects. The Speed-Dependent Hard Collision profile (SDHCP) [24], in which both effects are taken into account, is then used. Finally, the HTP which includes the correlation between velocity-changing and internal-state changing collisions in addition to the Dicke narrowing and to the speed-dependence effects, is also used in the analysis. Recall that, in Ref. [16], the best fits of some measured air-broadened CO<sub>2</sub> line shapes were obtained when taking this correlation into account. For the three speed-dependent profiles: SDVP, SDHC and HTP, the quadratic speed-dependence model of Ref. [25] was used (thus qSDVP and qSDHC for the acronyms of the profiles). Details of the functional forms and parameters can be found in [1] and references therein. During the fitting procedure, the area and the position of the line (including the speed-independent contribution of the line shift,  $\Delta_0$ ) as well as a linear base line were fitted separately for each pressure. The other parameters: the broadening coefficient  $\gamma_0$  ( $\Gamma_0/P$ ), its speed-dependent component  $\gamma_2$  ( $\Gamma_2/P$ ), the speed-dependent component of the line-shift coefficient  $\delta_2$  ( $\Delta_2/P$ ), the velocity-changing collisions frequency  $\nu_{vc}/P$ , and the correlation parameter  $\eta$  have a single value for all pressures.

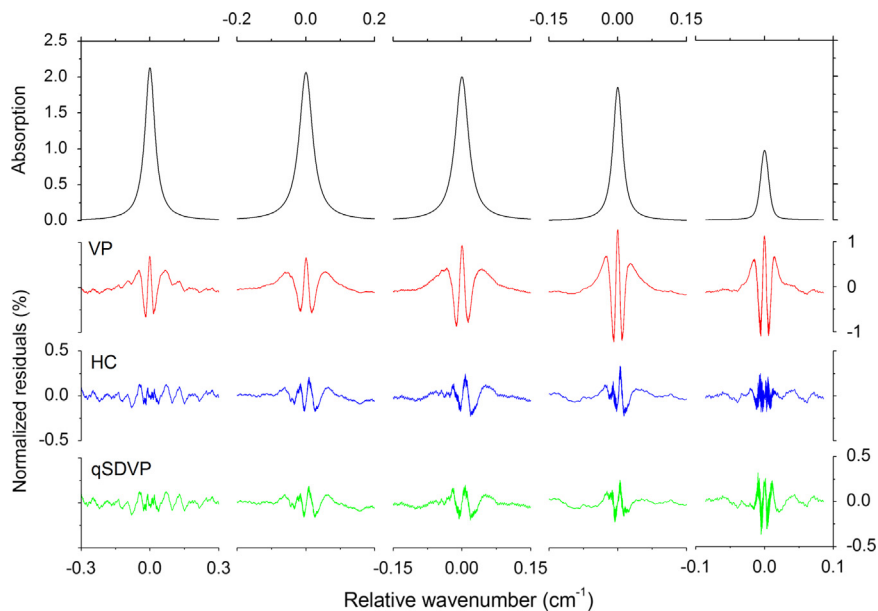
## 3. Results and discussions

Results obtained with a pressure-by-pressure (single-spectrum) fitting procedure are first presented in order to demonstrate the need to simultaneously adjust spectra measured at the various pressures. Fig. 1 shows examples of the fit residuals obtained for five pressures using this single-spectrum analysis with the VP, HCP and qSDVP. As expected, the VP gives the worst residuals. The HCP and qSDVP, although taking into account two different non-Voigt effects

**Table 1**

Pressure and optical path conditions used for the four studied lines. The line positions and Lorentz width ( $\Gamma_L$ ) are taken from Ref. [19].

Line	Position (cm <sup>-1</sup> )	Pressures (atm)	$\Gamma_L/\Gamma_D$ range	Optical path (m)
R(10)	6236.036992	0.226; 0.194; 0.163; 0.130; 0.105; 0.077; 0.053; 0.026; 0.013 0.130; 0.118; 0.079	4.1–0.2	16 8
R(12)	6237.421424	0.231; 0.197; 0.162; 0.132; 0.105; 0.078; 0.052; 0.025; 0.013 0.264; 0.194; 0.132; 0.118; 0.079; 0.066	4.7–0.2	16 8
R(20)	6242.672190	0.230; 0.196; 0.164; 0.127; 0.105; 0.079; 0.052; 0.026 0.591; 0.525; 0.458; 0.394; 0.328; 0.263; 0.197; 0.132; 0.119; 0.079; 0.066	10.2–0.4	16 8
P(38)	6313.002599	0.132; 0.105; 0.066; 0.051; 0.025 0.262; 0.227; 0.195; 0.164; 0.130; 0.119; 0.105; 0.078; 0.064 0.329; 0.263; 0.197	4.7–0.9	32 24 20



**Fig. 1.** Single-spectrum fits of the R(20) line for five pressures. From left to right: 0.263 atm; 0.230 atm; 0.164 atm; 0.105 atm; 0.025 atm. The upper panel shows the measurement while the three lower panels present the peak-absorption-normalized fit residuals obtained with the VP, HCP and qSDVP, respectively.

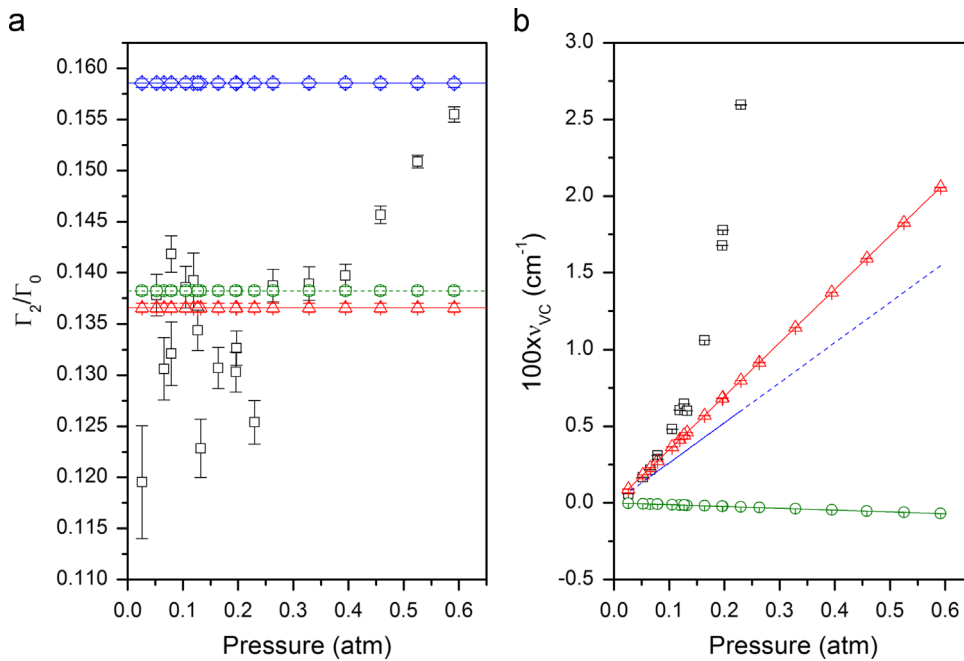
(i.e. Dicke narrowing and speed dependence, respectively), lead to similar results, much better than those obtained with the VP. Note that it was impossible to obtain convergence with profiles which take both effects into account using this single-spectrum fitting procedure, due to the strong correlation between the floated parameters.

Fig. 2 presents the pressure dependence of the ratio of the quadratic speed-dependent component to the line width  $\Gamma_2/\Gamma_0$  and that of the velocity-changing collisions frequency  $\nu_{VC}$  for the R(20) line as obtained by fitting the measured spectra one-by-one with the qSDVP and the HC models, respectively. As collisional parameters,  $\Gamma_0$ ,  $\Gamma_2$  and  $\nu_{VC}$  should be linear versus pressure and  $\Gamma_2/\Gamma_0$  should thus be independent of pressure. However, as can be observed in Fig. 2,  $\Gamma_2/\Gamma_0$  strongly depends on pressure while the collisional narrowing parameter  $\nu_{VC}$  shows a strong non-linear dependence with pressure. These results, previously observed in many other studies devoted to CO<sub>2</sub> and other molecules [13,16,26,27] demonstrate that these two models are not appropriate for the spectral shapes of CO<sub>2</sub> lines. Note that the theoretical value of  $\nu_{VC}/P$  (0.0264 cm<sup>-1</sup> atm<sup>-1</sup>, blue line in Fig. 2(b)), deduced from the diffusion coefficient [18], is rather small but not negligible when compared to the broadening coefficient of the considered CO<sub>2</sub> lines [19]. This demonstrates that the Dicke narrowing should contribute to the shape of these CO<sub>2</sub> lines. However, the non linearity of  $\nu_{VC}$  obtained with the HC model shows that this effect alone cannot explain all the non-Voigt effects observed in the line shapes of CO<sub>2</sub> at various pressures. Therefore, in the next step, profiles which take into account both the Dicke narrowing and the speed dependences of the line width and shift are used in the analysis with a multi-spectrum fitting technique. The latter allows to remove the correlation between  $\Gamma_2$  and  $\nu_{VC}$  since both the speed-dependence and the

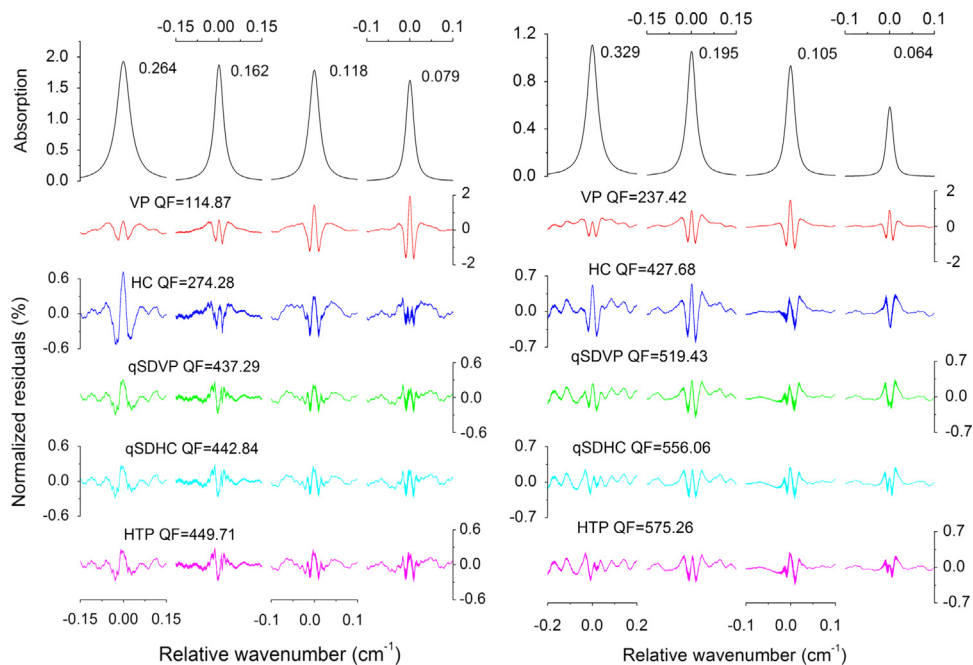
velocity-changes lead to a narrower line but not in the same pressure range.

Measured spectra at various pressures (see Table 1) are then simultaneously fitted with the qSDHC and the HTP but also with the above-mentioned simplified profiles (qSDVP, HCP, VP). Because of the large number of parameters in the HTP and of the correlation between some of them (e.g. between  $\eta$  and  $\Gamma_2$ ,  $\Delta_2$  as well as  $\nu_{VC}$ ) and the relatively low S/N ratio of the present measurements, it was impossible to fit all the parameters due to convergence problems. Note that this problem was already mentioned in Ref. [28]. Therefore, for the HTP, we have chosen in the following to fix the value of  $\nu_{VC}$  to its theoretical value as deduced from the diffusion coefficient of CO<sub>2</sub>.

Fig. 3 shows examples of the fit residuals obtained using the multi-spectrum fitting technique for the five considered line-shape models. The values of the quality fit (QF, ratio of the peak absorption to the standard deviation of the fit residuals [29]) for each model are also reported. As expected, the Voigt profile leads to the largest residuals and to the worse quality fit. The results of the HCP are almost two times better than those of the VP and the qSDVP is significantly better than the HCP. This conclusion was also obtained for transitions of many other systems such as air-broadened CO<sub>2</sub> [16], self-broadened H<sub>2</sub>O [30–32], H<sub>2</sub>O perturbed by N<sub>2</sub> and SF<sub>6</sub> [28], and self-broadened O<sub>2</sub> [33–35], molecular systems for which the value of  $\nu_{VC}$  is rather small when compared to that of the line broadening coefficient. These results suggest that the contribution of the speed dependence is more important than that of the velocity changes for these cases. Hence, fixing the value of  $\nu_{VC}$  to its theoretical value calculated from the diffusion coefficient should be an acceptable approximation for these systems. Finally, the qSDHC and HTP lead to very



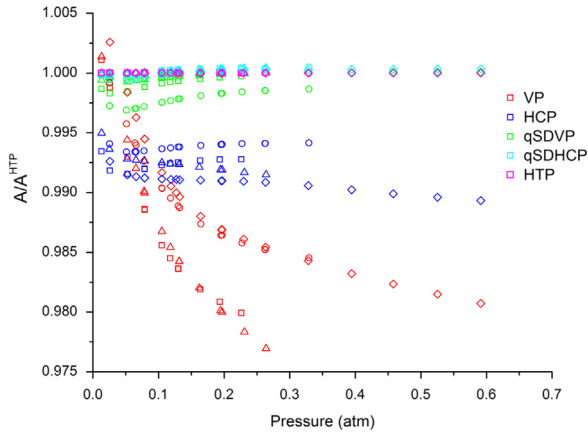
**Fig. 2.** Pressure dependences of the  $\Gamma_2/\Gamma_0$  ratio (a) and of the Dicke narrowing parameter (b) for the R(20) line, obtained from fits of measured spectra with the qSDVP and the HC model, respectively. Results obtained from single-spectrum and multi-spectrum analyses are plotted in black squares and red triangle symbols, respectively. The olive circles and blue diamonds are respectively the results obtained from multi-fitting the measured spectra with the qSDHC and HTP. Error bars represent the uncertainties resulting from the fits. The blue line in (b) is the theoretical value of  $v_{VC}$  calculated from the diffusion coefficient. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 3.** Examples of measured spectra (top panel, with the corresponding pressure in atm for each spectrum) and residuals obtained by the multi-spectrum fitting technique with various line-shape models. The left and right panels display the results obtained for the R(12) and P(38) lines, respectively.

similar residuals, slightly better than that of the qSDVP. This is also consistent with the results of Ref. [28] for H<sub>2</sub>O in N<sub>2</sub> where it was shown that with experimental S/N ratios below 1000, the qSDVP, qSDHC and the HTP lead to similar fit qualities. Better S/N ratios in the measurements

are needed if one wants to more clearly distinguish the qualities of fits obtained with the qSDVP, qSDHC and HTP. We note that the wave structures that are seen in the wings of the residuals when using the sophisticated models qSDVP, qSDHC and HTP are an experimental

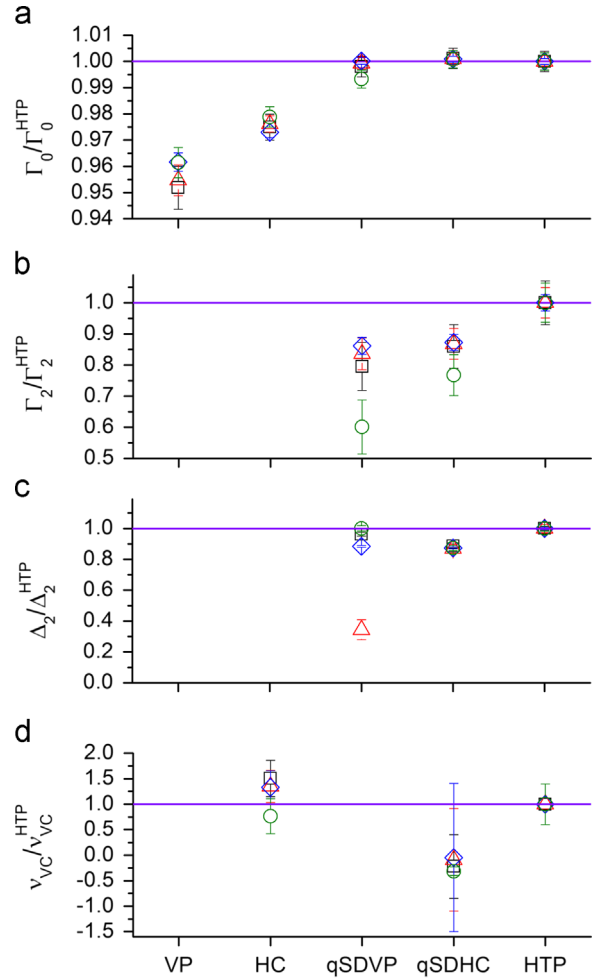


**Fig. 4.** Ratios of the line areas retrieved by multi-fitting (see text) the measured spectra with simplified profiles to those obtained with the HTP for the four considered lines. Results for the R(10), R(12), R(20) and P(38) are respectively represented by squares, triangles, diamonds and circles. The different colors are for different profiles. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

artifact caused by slight laser intensity drifts during the measurements.

Comparisons between the parameters obtained from multi-spectrum fits of measured spectra using various simplified profiles and those retrieved with the HTP are presented in Figs. 4 and 5 for the four considered lines. These display the line area, the collisional line width, its quadratic speed-dependent contribution, the quadratic speed-dependence of the line shift and the velocity-changing collision frequency. Since the line areas were fitted individually for each pressure, the ratios of the values retrieved with simplified models to those obtained with the HTP are thus plotted versus pressure in Fig. 4. As can be observed, when compared to the HTP, the results of the VP differ by up to 2.5% for the line area. These differences are about two times smaller when the HCP is used. The three speed-dependent profiles lead to similar areas except for the qSDVP at low pressures where differences up to 0.5% can be observed. This is probably due to the contribution of the Dicke narrowing effect, neglected in the qSDVP. These results for the line area are qualitatively consistent with the fit residuals observed in Fig. 3.

For the collisional broadening parameter  $\Gamma_0$ , the three speed-dependent profiles lead to very close values while with the VP and the HCP the differences are about 5 and 3% respectively. The quadratic speed-dependent parameter  $\Gamma_2$  given by the qSDVP is very different from that obtained with the HTP, especially for the P(38) line with a difference of about 40%. This is likely due to the fact that the Dicke narrowing and the correlation between velocity changes and internal-states changes are neglected in the qSDVP. For the velocity-changing collision frequency  $\nu_{VC}$ , the value obtained by the qSDHC model is negative and very close to the quantity  $(\nu_{VC}^{HTP} - \eta\Gamma_0)$ , obtained with the HTP. This unphysical behavior of  $\nu_{VC}$ , also observed previously for O<sub>2</sub> [35] when using the qSDHC, demonstrates that the correlation between velocity-changing and



**Fig. 5.** Ratios of the fitted line-shape parameters obtained with simplified profiles to those obtained with the HTP for the four considered lines: (a) collisional line width  $\Gamma_0$ , (b) quadratic speed-dependent contribution to the line width  $\Gamma_2$ , (c) quadratic speed-dependent contribution to the line shift  $\Delta_2$ , (d) velocity-changing collision frequency  $\nu_{VC}$ . In black squares, red triangles, blue diamonds and green circles are the results for the R(10), R(12), R(20) and P(38) lines, respectively. Error bars represent the uncertainties obtained from the fits. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

internal state-changing collisions cannot be neglected in these cases.

The various line-shape parameters obtained with the HTP for the four considered lines are presented in Table 2. The combined standard uncertainties are also reported for all the parameters. Note that the optical path and the absolute frequency are not known with high precision so that the values of the line intensity and line shift are not reported.

#### 4. Conclusions

Spectra of four self-broadened CO<sub>2</sub> lines near 1.6  $\mu\text{m}$  have been measured with a tunable diode laser spectrometer and analyzed using the recently recommended HT profile as well as some more simplified line-shape models.

**Table 2**

Line-shape parameters obtained from multi-spectrum fits of measured spectra with the HTP: collisional broadening coefficient  $\gamma_0$ , quadratic speed-dependent components of collisional broadening  $\gamma_2$  and shifting  $\delta_2$ , correlation between velocity- and internal state-changing collisions  $\eta$ . The value of the velocity-changing collisions frequency  $\nu_{VC}$  is fixed at the value calculated from the diffusion coefficient. The unperturbed line positions are taken from HITRAN [19].

Line	Position (cm <sup>-1</sup> )	$\gamma_0$ (cm <sup>-1</sup> atm <sup>-1</sup> )	$\gamma_2$ (cm <sup>-1</sup> atm <sup>-1</sup> )	$\delta_2$ (cm <sup>-1</sup> atm <sup>-1</sup> )	$\nu_{VC}/P$ (cm <sup>-1</sup> atm <sup>-1</sup> )	$\eta$
R(10)	6236.036992	0.1108(4)	0.0187(11)	-0.0010(3)	0.02614	0.295(60)
R(12)	6237.421424	0.1069(4)	0.0165(9)	0.0003(1)	0.02614	0.273(54)
R(20)	6242.672190	0.1004(4)	0.0159(10)	0.0007(1)	0.02614	0.273(54)
P(38)	6313.002599	0.0866(3)	0.0145(8)	-0.0006(1)	0.02614	0.423(84)

A multi-spectrum fitting technique has been used for the analysis of the measured spectra. The results show that the usual Voigt profile leads to large deviations with respect to the measured line shapes and causes significant errors on the retrieved line area. For the considered transitions, the speed-dependence effects seem to be the dominant narrowing mechanism when compared to the collision-induced velocity changes. Thanks to the broad pressure ranges of the measurements and to the multi-spectrum analysis, it is shown that both the Dicke narrowing and the speed dependence must be simultaneously considered to correctly describe the measured spectra. Taking the correlation between velocity- and internal-state changing collisions into account is necessary to obtain physically-meaningful value for the velocity-changing collision frequency. Among all the line-shape models used, the HT profile is the most appropriate one for the modeling of the shape of all the considered lines since it leads to the best agreement with the measurement and physically-based line-shape parameters.

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