

Measurements and predictions of H₂ pressure-broadening coefficients of CO₂ absorption lines for exoplanet atmosphere studies

Faten Hendaoui^{1,2}, Pascale Chelin³ , Xavier Landsheere³, Hassen Aroui², and Ha Tran^{1,*} 

¹ Laboratoire de Météorologie Dynamique, IPSL, Sorbonne Université, École Normale Supérieure, Université PSL, École polytechnique, Institut Polytechnique de Paris, CNRS, Paris, France

² Université de Tunis, Laboratoire de Spectroscopie et Dynamique Moléculaire, École Nationale Supérieure d'Ingénieurs de Tunis, 5 Av. Taha Hussein, 1008 Tunis, Tunisia

³ Univ Paris Est Créteil and Université Paris Cité, CNRS, LISA, F-94010 Créteil, France

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ABSTRACT

Accurate and comprehensive H₂ pressure-induced broadening data for CO₂ infrared lines over a wide temperature range are essential for modeling atmospheric opacity of exoplanets. However, available data are currently limited, some of which are affected by large uncertainties. In this work, H₂ pressure-induced broadening and pressure-shift coefficients were determined at room temperature for the entire ν_3 band of CO₂ in the 4.3 μm spectral region using a high-resolution Fourier transform spectrometer. In addition, requantized molecular dynamics simulations of the CO₂-H₂ system were performed using an accurate intermolecular potential. These simulations provide theoretical predictions of H₂ broadening coefficients for CO₂ lines over a temperature range of 200–1000 K and for rotational quantum number up to $J = 120$. The predicted results show very good agreement with the experimental data, with difference of less than 3%, well below the precision required for exoplanet atmosphere studies. This work provides the first accurate and comprehensive dataset of H₂ broadening coefficients for CO₂ lines, suitable for modeling of H₂-rich exoplanetary atmospheres.

Key words. line: profiles – molecular data – opacity – radiative transfer – methods: laboratory: molecular – techniques: spectroscopic

1. Introduction

Reliable H₂ pressure-broadening data for a variety of molecules and under wide temperature conditions are essential for accurately modeling exoplanetary atmospheres (Hedges & Madhusudhan 2016; Fortney et al. 2019; Tan et al. 2022). The accuracy of molecular abundances, or more generally atmospheric properties, derived from measured spectra depends on the precision of molecular cross sections, which relies on the knowledge of molecular spectroscopic data, including line position, line intensity, pressure-induced line broadening, and shift due to collisions between the optically active molecule and the main constituents of the considered atmosphere. Several studies demonstrated that the lack of pressure-broadening data leads to large impacts on opacity modeling and the retrieval of atmospheric properties for planets and exoplanets (e.g., Hedges & Madhusudhan 2016; Gharib-Nezhad & Line 2019; Garland & Irwin 2019; Wiesenfeld et al. 2025).

However, reliable pressure-broadening information under exoplanet thermophysical conditions remains scarce due to the wide variety of constituents, and temperature and pressure conditions that must be considered. In the absence of available experimental and theoretical data, air-broadened widths are often used with empirical scaling factors (Wilzewski et al. 2016; Tan et al. 2019, 2022) to describe the broadening by the main interfering gases in exoplanetary atmospheres such as H₂ and He. This approach can cause significant discrepancies

when compared to accurate measured or calculated broadening data (see Hendaoui et al. 2026, for instance). Furthermore, the temperature range encountered in exoplanet atmospheres extends far beyond that of the Earth's atmosphere. For instance, Fortney et al. (2019) noted that for H₂- and He-dominated exoplanet atmospheres, the temperature of interest spans from 70 K to 3000 K.

Carbon dioxide (CO₂) is a key molecule in exoplanetary atmospheres. It is detected in a wide range of planets observed with the James Webb Space Telescope (JWST; e.g., Ahrer et al. 2023; Balmer et al. 2025). The prominent 4.3 μm absorption feature is especially valuable as it lies in a spectral region with minimal noise and cloud-haze interference, making it of great interest for both detection and habitability assessments (see Wiesenfeld et al. 2025 and references therein). Exploiting this feature is, however, limited by incomplete opacity models, particularly uncertainties in line-broadening and far-wing parameterizations (Niraula et al. 2022). Wiesenfeld et al. (2025) showed that a precision on pressure-broadening coefficients of better than 10% is required for JWST exoplanet studies.

Despite their importance, there are few studies devoted to the measurement or calculation of the H₂ pressure-broadening coefficients for CO₂ lines. In Padmanabhan et al. (2014), H₂ broadening coefficients were measured at room temperature for ten CO₂ lines, ranging from P(16) to P(34), in the 6317–6335 cm⁻¹ region of the 30012←00001 band, using a tunable diode laser. These coefficients were derived from spectra measured for mixtures of CO₂, N₂, and H₂, with a stated uncertainty of

* Corresponding author: htran@lmd.ipsl.fr

about 6%. The measured coefficients vary significantly with the rotational quantum number, from $0.095 \text{ cm}^{-1}/\text{atm}$ for the P(32) line to $0.121 \text{ cm}^{-1}/\text{atm}$ for the P(20) line. However, no clear rotational dependence is observed, indicating that the actual uncertainty is probably larger than 6%. Hanson and Whitty (Hanson & Whitty 2014) measured the H_2 broadening coefficient for the P(24) line of CO_2 at 4957.08 cm^{-1} , using wavelength-scanned spectroscopy. These measurements were taken at various temperatures, from 300 K to 700 K, with an uncertainty claimed to be better than 2%. Their room temperature value for the P(24) line is $0.112 \text{ cm}^{-1}/\text{atm}$, which closely matches the value of $0.1128 \text{ cm}^{-1}/\text{atm}$ reported by Padmanabhan et al. (2014) for the same line. Hanson and Whitty also deduced a temperature dependence exponent of 0.582 for this P(24) line. The experimental investigation by Burch et al. (1969) suggested that H_2 broadening is 1.17 times larger than self-broadening for CO_2 lines, with the same rotational dependence assumed for broadening by various collision partners. These limited data have been used in various radiative transfer models to calculate the optical thickness of exoplanet atmospheres (e.g., Tremblin et al. 2015; Goyal et al. 2017; Garland & Irwin 2019).

More recently, Wiesenfeld et al. (2025) conducted ab initio calculations of H_2 pressure broadening for the P(24) line of CO_2 in the ground vibrational state. They found that their calculations agree with the measured values of Padmanabhan et al. (2014); Hanson & Whitty (2014) within 7%. Nie et al. (2025) measured room temperature H_2 broadening coefficients for four CO_2 lines in the $20012\leftarrow 00001$ band, from R(44) to R(50) using a distributed feedback laser. H_2 broadening coefficients of CO_2 lines in the HITRAN database (Gordon et al. 2021) were simply obtained using a scaling factor of 1.5767 on the air-broadening coefficients. Additionally, a constant temperature dependence exponent of 0.58 was applied to all CO_2 transitions in HITRAN. It is evident that more accurate and comprehensive measurements and calculations are necessary to provide more reliable line-shape data for this system.

In order to provide a reliable and comprehensive dataset for H_2 broadening coefficients of CO_2 lines relevant for exoplanet atmosphere studies, we conducted high-resolution laboratory measurements and first-principle calculations. Specifically, a high-resolution Fourier transform spectrometer was used to record spectra of CO_2 highly diluted in H_2 in the $4.3 \mu\text{m}$ spectral range, at room temperature and pressures ranging from 150 mbar to 1060 mbar. The recorded spectra were then analyzed to extract both the pressure-broadening coefficients and the pressure-induced shifts of 61 CO_2 lines, from P(62) to R(60). A detailed uncertainty analysis was performed on the obtained parameters, considering uncertainties from various sources. This study represents the first measurement of these coefficients for an entire ro-vibrational band of CO_2 . In the second step, we used requantized classical molecular dynamics simulations (rCMDs) to predict CO_2 line broadening by H_2 over a broad temperature range, from 200 K to 1000 K, which is highly relevant for opacity modeling in exoplanetary atmospheres. These simulations, based on the use of accurate intermolecular potentials and classical theory of molecular collisions, have previously demonstrated the ability to reproduce self-, air-, and He-broadened CO_2 line-shape parameters (Ngo & Tran 2025; Tran et al. 2025; Hendaoui et al. 2026) with relative errors well below 5% for rotational quantum numbers up to $J=160$ and temperatures as high as 3000 K.

The paper is organized as follows. Section 2 focuses on the experimental determination of the pressure-induced line broadening and shift. Section 2.1 describes the experimental setup,

Table 1. Pressures and temperatures of the recorded spectra.

Spectrum number	P_{CO_2} (mbar)	P_{tot} (mbar)	T (K)
1	0.0803	0.0803	293.50
2	0.0723	150.65	293.50
3	0.1460	506.89	293.80
4	0.2205	756.73	294.25
5	0.2804	1062.04	293.30

the measurement procedure, and the determination of the instrument line shape. The fitting procedure and uncertainty analysis are detailed in Sect. 2.2. The obtained line-broadening and pressure-shift parameters are presented and compared with available data in Sect. 2.3. The rCMDs first-principle calculations for $\text{CO}_2\text{-H}_2$ are described in Sect. 3. Section 3.1 details the calculation methods and procedures. The predicted broadening coefficients are then presented and compared with measured values in Sect. 3.2, while the temperature dependence of line broadening is described in Sect. 3.3. Finally, in Sect. 4 we present the conclusions of this work.

2. Measurements

2.1. Experimental setup and recording procedure

The high-resolution Fourier transform spectrometer (FTS) at LISA (Bruker IFS-125 HR) was used to record all spectra. The instrument was equipped with a silicon carbide Globar source, a KBr/Ge beamsplitter, and a liquid nitrogen cooled indium antimonide (InSb) detector. The diameter of the FTS iris aperture was set to 2 mm and the focal length of the collimator was 418 mm. No artificial optical weighting was performed (a box-car function was selected). A 12.3 cm simple-pass absorption cell was used. The Bruker spectral resolution was 0.01 cm^{-1} , corresponding to a maximum optical path difference of 90 cm.

The measurements were carried out as follows. The cell was first filled with a very small quantity of CO_2 (measured with a 2-Torr full-scale Baratron gauge, MKS 627D model, with an accuracy of 0.15% of reading) and then completed with H_2 to reach the desired total pressure. The latter was measured with a 1000-Torr full-scale Baratron gauge, MKS 628D model, with a stated accuracy of 0.25% of reading. Commercial carbon dioxide and hydrogen samples from Air Liquide were used without purification (99.9% natural CO_2 ; 99.9999% H_2). After approximately 20 minutes, once the mixture was homogeneous, a spectrum was recorded by co-adding 3200 scans over a period of 24 hours. The cell was then pumped out and refilled to reach the next desired total pressure. This procedure was adopted to limit any leakage of ambient air into the cell during measurement. The variation in total pressure during 24-hour acquisition was approximately 0.3 mbar (with a mean leak of $2.12 \cdot 10^{-4} \text{ mbar/min}$). The average temperature during the recordings was about 293.71 K, with a mean variation of 0.3 K per recording (room temperature was used as a proxy for cell temperature). In total, four spectra of mixtures with total pressure ranging from 150 mbar to 1060 mbar were recorded with spectral range spanning from 2200 cm^{-1} to 2500 cm^{-1} . This spectral region covers the entire $\text{CO}_2 \nu_3$ band of interest. The experimental pressures and temperatures of the recorded spectra are summarized in Table 1.

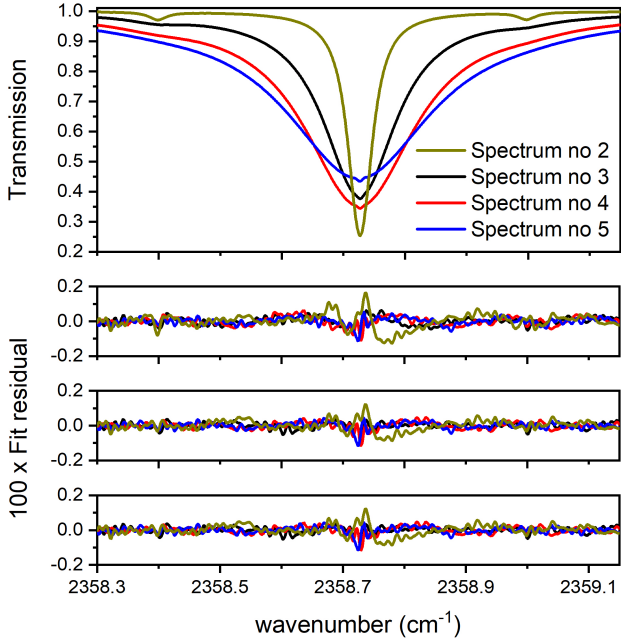


Fig. 1. Measured transmission of the R(12) line (top panel) and fit residuals obtained by fitting the measured spectra with the Voigt profile (second panel), with LM accounted for (third panel) and with the HC model together with LM (bottom panel).

Two empty-cell spectra were recorded with the same optical conditions after pumping down to a pressure below 10^{-4} mbar. These provided the 100% transmission baseline by removing remaining traces of H_2O and CO_2 inside the interferometer, and enabled partial removal of the multiplicative channel due to interferences arising from the parallel faces of the cell windows. For each pressure, the corresponding spectrum was obtained by dividing the spectrum recorded with gas by the empty-cell spectrum. A signal-to-noise ratio up to ~ 1500 (see Figure 1) was achieved for the transmission spectra.

A pure CO_2 spectrum at 0.08 mbar was also recorded to determine the instrument line shape (ILS) using the LINEFIT 14.8 software (Hase et al. 1999; Hase 2012). The results show small asymmetry on the ILS and a modulation close to 1, demonstrating that the different optics of the instrument were well aligned. We performed several tests to determine the optimal spectral interval and sampling step for the ILS.

For spectral calibration, we used CO_2 lines appearing in the empty-cell spectra due to small residual amounts of CO_2 inside the FTS. The positions of eight intense lines, determined from fits using a Gaussian profile, were compared with the corresponding line positions given in the HITRAN database (Gordon et al. 2021). The resulting calibration factor was 1.000000467, the standard deviation of the fitted positions being about $2 \times 10^{-5} \text{ cm}^{-1}$. As discussed below, because the contribution of weak lines is fixed in the fits using HITRAN spectroscopic line position, accurate spectral calibration is important.

It should be noted that, due to the very small quantity of CO_2 introduced (see Table 1), possible partial adsorption of the gas on the cell walls, and minor leaks during gas filling, the CO_2 partial pressure in the mixture is not known with high precision. However, since the absolute line intensity is not the focus of this work and because the amount of CO_2 is very small, the uncertainty in the CO_2 pressure does not affect the measured H_2 pressure-induced line shape of the considered CO_2 transitions.

2.2. Spectra analysis and uncertainty determination

The measured transmission spectrum of CO_2 broadened by H_2 can be expressed as:

$$T(\sigma, P_{\text{CO}_2}, P_{\text{H}_2}, T) = \exp \left[-L P_{\text{CO}_2} \sum_i S_i(T) \phi(\sigma - \sigma_i, P_{\text{CO}_2}, P_{\text{H}_2}, T) \right] \otimes \text{ILS} \quad (1)$$

where the symbol \otimes indicates the convolution between the high-resolution transmission with the instrument line-shape function, L (cm) is the absorption path length, and P_{CO_2} and P_{H_2} (atm) are respectively the CO_2 and H_2 pressures in the mixture. The sum is over all lines contributing to absorption at wavenumber σ (cm^{-1}). The quantity $S_i(T)$ ($\text{cm}^{-2} \text{ atm}^{-1}$) is the intensity of the line i at temperature T (K) and $\phi(\sigma - \sigma_i, P_{\text{CO}_2}, P_{\text{H}_2}, T)$ (in cm) is the line shape or the normalized profile of this line. In the simplest case, this line-shape function is expressed by the Voigt profile, which is a convolution of a Gaussian and a Lorentzian profile, taking into account respectively the Doppler broadening and pressure-induced broadening and shift of the line. More sophisticated models can be used for ϕ as well, taking into account more refined pressure-induced collisional effects such as the speed dependence of the line broadening and shift, the Dicke narrowing, and the collision-induced interferences between line (i.e., line mixing) (Ngo et al. 2013; Wcisło et al. 2025).

Here we used three different profiles to fit the measured spectra: the usual Voigt profile, the Voigt profile with line mixing (LM) accounted for, and the hard-collision (HC) profile with LM. The Doppler width was calculated for the temperature of the measurement of each spectrum and fixed in the fits. For the Voigt profile, two line-shape parameters were fitted: the H_2 pressure-broadening coefficient, γ_{H_2} , and the H_2 pressure shift, δ_{H_2} (both in $\text{cm}^{-1}/\text{atm}$). To model the weak LM effects between CO_2 lines at the considered pressures, we used the first-order approximation (Rosenkranz 1975). In this case, the LM coefficient, ξ (atm^{-1}), is also adjusted. Finally, to model the weak Dicke narrowing effect, due to molecule velocity changes caused by collisions, we used the hard-collision model (Nelkin & Ghatak 1964), leading to an additional parameter to be fitted, the Dicke narrowing parameter, or the velocity changing rate, ν_{VC} ($\text{cm}^{-1}/\text{atm}$). When the signal-to-noise ratio of the measured spectra is high enough, refined line-shape models lead to better agreement with measurements. The retrieved line-broadening coefficient also slightly depends on the used line shapes (see Ngo et al. 2013 and references therein).

A multi-fitting procedure was used, in which we fitted simultaneously the four measured spectra of CO_2 in H_2 , constraining the different line-shape parameters (i.e., γ_{H_2} , δ_{H_2} , ξ , and ν_{VC}) to be the same at different pressures. The instrument line-shape function, determined from the pure CO_2 spectrum measured at low pressure, as explained in Sect. 2.1, was fixed in the fits. In addition to the line-shape parameters, the line area [i.e., $L^*P_{\text{CO}_2} * S_i(T)$] and line position (at zero pressure) were also fitted. Spectral ranges about 2 cm^{-1} were considered at a time in the fits. All lines with integrated intensity greater than $1 \times 10^{-20} \text{ cm}^{-1}/(\text{molec} \cdot \text{cm}^{-2})$ were fitted. These correspond to lines of the ν_3 band of the main isotopologue of CO_2 with rotational quantum number J up to 62. The contribution of weaker lines was calculated for the measured experimental conditions using spectroscopic data from the HITRAN database (Gordon et al. 2021), except for the line broadening coefficient. The latter was estimated from the first round fits of the ν_3 lines of $^{12}\text{CO}_2$

and neglecting any vibrational and isotopic dependences of the broadening coefficient. For the calculation of weak lines, the partial pressures of CO₂ for each spectrum was redetermined using the fitted areas and integrated intensities in HITRAN for several strong ν_3 lines of ¹²CO₂. For each spectral range and pressure, we used two baseline models for the 100% transmission: a linear baseline and a third-order polynomial function. The parameters of the baseline were also fitted. The difference in the retrieved line-shape parameters obtained with these two baseline models was accounted for in the estimation of their uncertainties.

Examples of the measured transmissions and the corresponding fit residuals obtained with the three line-shape models are shown in Fig. 1. The residuals obtained with LM taken into account are close to the experimental noise level; the weak remaining residuals are probably due to the imperfect modeling of the instrument line shape. It was not possible to fit all lines with the HC model with first-order LM, probably due to the limited signal-to-noise ratio of the measured spectra. This model resulted in only marginally better fit residuals compared to those obtained with the Voigt model with LM. In addition, the differences between the γ_{H_2} values obtained with Voigt+LM and HC+LM are well below the total uncertainty. We note that a similar conclusion was obtained when using the speed-dependent Voigt profile (Ngo et al. 2013) to fit the measured spectra. Therefore, in the following, we focus and discuss results obtained with Voigt+LM only.

The uncertainty of the fitted parameters comes from different sources. The first is the statistical uncertainty (type A), corresponding to the standard deviation obtained from the fits. This quantity is negligibly small compared to the systematic uncertainties. The latter arise from the uncertainty in the measured pressure and temperature, and in the apparatus function. In our analysis, we assumed that self-broadening effects are the same as H₂ broadening effects, i.e., $P_{\text{H}_2} = P_{\text{tot}}$. This assumption has a largely negligible effect on the determined H₂ collision-induced line-shape parameters since the concentrations of CO₂ in the mixtures are low (see Table 1). To determine the uncertainty due to errors in the measured P_{tot} , we reanalyzed the four measured spectra, but with the total pressure $P_{\text{tot}} = P_{\text{tot}}^{\text{meas}} + \Delta P$, where ΔP is the error in the measured total pressure. The corresponding uncertainty of the line-shape parameters was then determined as the difference between the parameters obtained using ($P_{\text{tot}}^{\text{meas}} + \Delta P$) and those obtained using $P_{\text{tot}}^{\text{meas}}$. A similar procedure was performed to determine the uncertainty due to the uncertainty of the measured temperature. In addition, the line-shape parameters were considered as being obtained at the average temperature. The uncertainty due to the difference between the average temperature and the temperature measured for each spectrum was also considered, using the temperature dependence exponent of H₂ broadening coefficients provided in the HITRAN database (Gordon et al. 2021). Uncertainties due to errors in the ILS were estimated by performing fits with two ILSs, both determined using LINEFIT, by applying LINEFIT to selected microwindows and to the entire R branch in the pure CO₂ spectrum. The total uncertainty for each retrieved parameter was then computed as the sum of all individual contributions, including that arising from the choice of baseline models. Except for a few lines of high rotational quantum number, this computed uncertainty is below 2%. We therefore assume that the total uncertainty of the measured γ_{H_2} for these lines is 2%.

2.3. Results and comparison with available data

The obtained values of γ_{H_2} are listed in Table 2, and are plotted in Fig. 2 as a function of $|m|$, where $m = -J$ and $m = J+1$

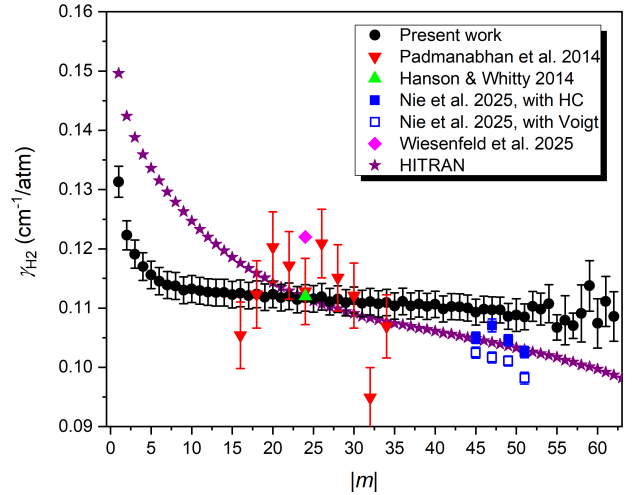


Fig. 2. H₂ broadening coefficient measured in this work, and a comparison with the available experimental and theoretical data and with the values from HITRAN (Tan et al. 2022).

in the P and R branches, respectively. The data available in the literature are also displayed in Fig. 2 for comparison. As can be observed, for the P(24) line, our result is in very good agreement with that of Hanson & Whitty (2014), with a difference of 0.25%. The calculated value of Wiesenfeld et al. (2025) for the same line is about 9% larger than our result. Larger discrepancies, up to 15%, are observed when comparing our values with those of Padmanabhan et al. (2014). In the latter study, a large and apparently random variation of γ_{H_2} with $|m|$ is observed, which is not the case for our data. Differences of up to 9% and 5% are observed when comparing our results with those of Nie et al. (2025) obtained with the Voigt and the HC profiles, respectively. We note that Nie et al. (2025) determined line intensity and broadening coefficients from spectra measured for mixtures of CO₂ with various perturbers such as O₂, N₂, H₂, and Ar. Their retrieved line intensity depends strongly on the perturber, with variation up to 3.2%, indicating large uncertainty in the retrieved parameters. Therefore, the actual uncertainty in the measured broadening must be significantly larger than the 1% uncertainty claimed. Finally, significant differences of up to 16.5% are also found when comparing our results with the values provided in HITRAN (Tan et al. 2022). The γ_{H_2} values in HITRAN were obtained by simply scaling the air-broadening coefficient to match the results of Hanson & Whitty (2014) at $|m| = 24$ (Tan et al. 2022). Our results therefore demonstrate that the rotational dependence of γ_{H_2} differs significantly from that of γ_{air} . Consequently, using these data (Padmanabhan et al. 2014; Tan et al. 2022) for opacity modeling of planetary and exoplanetary atmospheres may lead to substantial errors.

The measured pressure-shift coefficients, δ_{H_2} , are plotted in Fig. 3 versus the rotational quantum number. This work provides the first determination of δ_{H_2} for the ν_3 band. It is important to emphasize that δ_{H_2} were obtained by fitting the measured spectra accounting for LM effects. When a simple Voigt profile is used (neglecting LM), the derived coefficients differ significantly and exhibit a strong rotational dependence (see Fig. 3). This behavior is due to the influence of line-mixing effects, which can shift the peak absorption. As can be seen, the rotational dependence of δ_{H_2} is weak, similarly to what was observed for CO₂ broadened by He (Hendaoui et al. 2026), although the magnitude of δ_{H_2} is significantly larger. The mean value of δ_{H_2} is $-3.9 \cdot 10^{-3} \text{ cm}^{-1}/\text{atm}$, compared to $-0.52 \cdot 10^{-3} \text{ cm}^{-1}/\text{atm}$ for He. To

Table 2. H₂ pressure-broadening and pressure-shift coefficients of CO₂ lines in the ν_3 band measured around 294 K.

m	γ_{H_2}	δ_{H_2}	m	γ_{H_2}	δ_{H_2}
-62	0.1086 (42)	–	1	0.1313 (26)	-0.0045 (6)
-60	0.1074 (41)	–	3	0.1191 (24)	-0.0035 (6)
-58	0.1091 (48)	–	5	0.1156 (23)	-0.0047 (4)
-56	0.1079 (42)	–	7	0.1139 (23)	-0.0036 (4)
-54	0.1107 (32)	–	9	0.1130 (23)	-0.0032 (6)
-52	0.1103 (25)	-0.0047 (10)	11	0.1129 (23)	-0.0031 (7)
-50	0.1088 (27)	–	13	0.1126 (23)	-0.0025 (3)
-48	0.1097 (25)	-0.0050 (11)	15	0.1123 (22)	-0.0029 (6)
-46	0.1098 (22)	-0.0049 (5)	17	0.1121 (22)	-0.0031 (6)
-44	0.1100 (22)	-0.0045 (6)	19	0.1125 (22)	-0.0032 (8)
-42	0.1102 (22)	-0.0048 (6)	21	0.1117 (22)	-0.0031 (6)
-40	0.1106 (22)	-0.0042 (6)	23	0.1114 (22)	-0.0025 (4)
-38	0.1107 (22)	-0.0042 (4)	25	0.1115 (22)	-0.0031 (6)
-36	0.1111 (22)	-0.0046 (4)	27	0.1110 (22)	-0.0032 (7)
-34	0.1109 (22)	-0.0041 (6)	29	0.1109 (22)	-0.0032 (7)
-32	0.1111 (22)	-0.0044 (6)	31	0.1108 (22)	-0.0028 (4)
-30	0.1113 (22)	-0.0043 (4)	33	0.1107 (22)	-0.0031 (6)
-28	0.1115 (22)	-0.0047 (4)	35	0.1103 (22)	-0.0034 (7)
-26	0.1119 (22)	-0.0053 (5)	37	0.1104 (22)	-0.0033 (6)
-24	0.1117 (22)	-0.0043 (4)	39	0.1103 (22)	-0.0029 (3)
-22	0.1120 (22)	-0.0041 (6)	41	0.1099 (22)	-0.0033 (7)
-20	0.1123 (22)	-0.0044 (4)	43	0.1102 (22)	-0.0035 (6)
-18	0.1123 (22)	-0.0049 (6)	45	0.1093 (22)	-0.0029 (4)
-16	0.1125 (22)	-0.0042 (6)	47	0.1097 (22)	-0.0034 (5)
-14	0.1126 (23)	-0.0045 (7)	49	0.1086 (22)	-0.0034 (8)
-12	0.1127 (23)	-0.0042 (6)	51	0.1085 (22)	-0.0042 (7)
-10	0.1132 (23)	-0.0047 (6)	53	0.1098 (27)	-0.0031 (7)
-8	0.1137 (23)	-0.0045 (8)	55	0.1067 (21)	-0.0039 (11)
-6	0.1145 (23)	-0.0042 (8)	57	0.1070 (21)	-0.0044 (3)
-4	0.1170 (23)	-0.0041 (6)	59	0.1137 (43)	-0.0028 (24)
-2	0.1223 (24)	-0.0058 (9)	61	0.1111 (42)	–

Notes. These coefficients are expressed in $\text{cm}^{-1}/\text{atm}$. The number in parentheses indicates the corresponding uncertainty and has the same unit as the last significant digit.

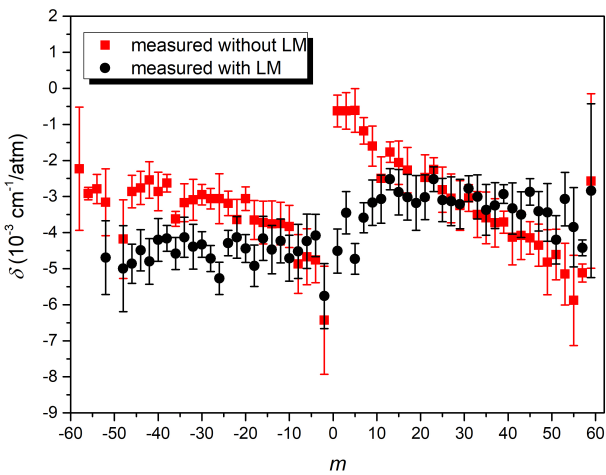


Fig. 3. H₂ pressure shift determined from fits of measured spectra with the Voigt profile (without LM) and with LM taken into account.

the best of our knowledge, the only previously available data on δ_{H_2} are those reported by Nie et al. (2025). In that study, H₂ pressure-induced shifts were measured for four CO₂ lines in the $\nu_1 + 2\nu_2 + \nu_3$ band, yielding a mean value of about $-7.5 \cdot 10^{-3} \text{ cm}^{-1}/\text{atm}$. The difference between their result and the

present measurements can be attributed to the strong vibrational dependence of the pressure-induced line shift.

3. Theoretical predictions of γ_{H_2}

3.1. Calculation method and data used

We employed rCMDs to predict γ_{H_2} over a broad temperature range, from 200 K to 1000 K. Using accurate intermolecular potentials and the Newtonian equations of motion, this method enables the simulation of the time evolution of a system containing a large number of molecules at a given pressure and temperature (Allen & Tildesley 1987). The auto-correlation functions (ACFs) of the dipole moment, responsible for the transitions, can thus be computed. The Fourier–Laplace transform of these ACFs directly yields the spectral density or the normalized spectral profile. In addition, we applied a requantization procedure (Hartmann et al. 2013) to the molecular rotation. The requantized spectral line obtained this way can then be fitted with a line-shape model, such as the usual Voigt profile, to deduce the corresponding pressure broadening. This approach has enabled very satisfactory predictions of line-shape parameters (Nguyen et al. 2018; Tran et al. 2019; Nguyen et al. 2020; Ngo et al. 2021; Hendaoui et al. 2024; Ngo & Tran 2025; Tran et al. 2025; Hendaoui et al. 2026), far-wing absorption (Hartmann et al. 2010, 2018), and

collision-induced absorption (Hartmann & Boulet 2011; Hartmann et al. 2017; Fakhardji et al. 2022) for various molecular systems and under wide ranges of pressure and temperature.

At the initial time, the molecules were positioned as follows: the center of mass of each molecule was randomly assigned, with a minimum separation of 7 Å to prevent unphysically strong interactions. The system then reaches equilibrium after a temperature- and pressure-dependent temporization time, t_{tempo} . Translational and angular speeds were initialized according to Maxwell–Boltzmann distributions, with random velocity vectors and molecular axis orientation assigned to each molecule. At each time step, the forces and torques acting on each molecule were computed to update their accelerations, translational velocities, position, angular velocities, and molecular orientations at the next time step $t + \Delta t$.

A requantization procedure (Hartmann et al. 2013) was applied to the classical rotation of the CO₂ molecules, but only when the interaction between the considered CO₂ molecule and its neighboring H₂ molecules was negligible. This approach, well suited for the CO₂ molecule due to the small energy separation between its rotational levels, was shown to yield excellent predictions of CO₂ broadening coefficients in N₂, O₂, He and self-broadening (Nguyen et al. 2018, 2020; Ngo & Tran 2025; Hendaoui et al. 2026). Specifically, for a molecule of rotational angular speed ω , the even integer J is determined such that $\frac{\hbar J}{I}$ is closest to ω , where I is the moment of inertia. This procedure matches the classical rotational frequency with the quantum position of the P-branch lines. Once J is found, ω is requantized by applying the change $\omega = \frac{\hbar J}{I}$, while the orientation of the rotational angular momentum remains unchanged. This P-branch requantization implies that the R-branch will be an exact mirror image of the P-branch.

The ACF of the dipole moment vector, assumed along the CO₂ molecular axis (as is the case for the asymmetric stretching absorption bands of CO₂), was then calculated during the rCMDSs. The Doppler effect associated with the translational motion was also included. Finally, the spectral profile (or the normalized absorption coefficient) was obtained from the Fourier–Laplace transform of the dipole moment ACF (Hartmann et al. 2021).

Here CO₂ molecules were modeled as linear rigid rotors in their equilibrium configuration, with all effects of vibrational motion disregarded in the calculations. This approximation is expected to have a negligible effect on the calculated pressure broadening (Hashemi et al. 2020). The CO₂–H₂ interaction was described using the site-site potential provided by Hellmann & Bich (2025). The parameters of this site-site potential, as well as the positions of the sites in the molecules were determined from the ab initio calculated interaction energies as described in Hellmann & Bich (2025). The spectra were thus calculated without using any parameter adjusted to the experimental data. We note that our rCMDSs do not account for dipole dephasing, which arises from different intermolecular interactions in the upper and lower states of the transitions. As a result, the calculated spectra do not show any pressure-induced vibrational shifts.

The simulations were performed on the Jean-Zay HPE SGI 8600 supercomputer at the Institut du Développement et des Ressources en Informatique Scientifique, which supports massively parallel computing. The molecules were distributed across four thousand boxes with periodic boundary conditions (Allen & Tildesley 1987), each containing 20 000 molecules. Mixtures containing 50% CO₂ were considered, but only CO₂–H₂ interactions were accounted for. This is equivalent to

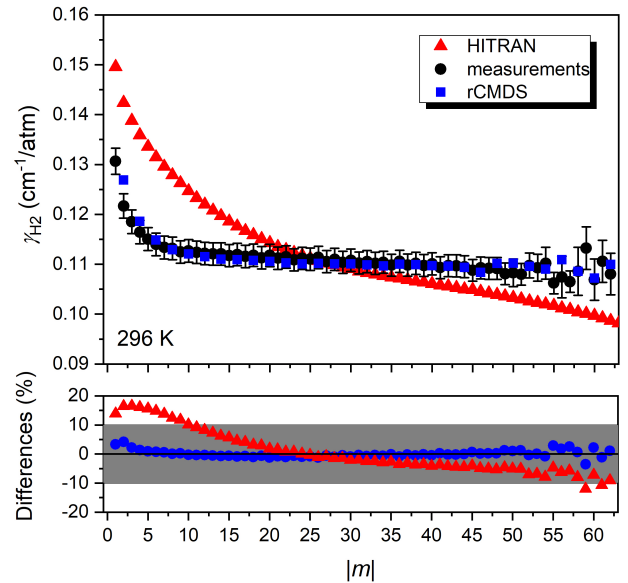


Fig. 4. H₂ broadening coefficient predicted by rCMDS at 296 K, and a comparison with the experimental values of the present work and with the HITRAN data. The gray space represents the 10% precision level required for exoplanetary atmosphere studies.

CO₂ being infinitely diluted in H₂, with the total pressure corresponding to the partial pressure of H₂. rCMDSs were performed for the following temperatures: 200 K, 296 K, 400 K, 500 K, 600 K, 800 K, and 1000 K. For each temperature, the pressure of the mixture was chosen such that line-mixing effects were negligible (pressures up to 0.5 atm for $T \leq 400$ K and up to 1 atm for T between 500 K and 1000 K). For each temperature, a total number of 8×10^7 molecules was considered, yielding signal-to-noise ratios of the calculated spectra of up to 1000 for the most intense lines.

Spectra calculated with rCMDS were fitted with Voigt profiles to retrieve the pressure-broadening coefficients. The line position, line area, and a linear baseline were also fitted, as for the measured spectra. Additional fits were performed using more refined models, such as the speed-dependent Voigt and HC profiles, to account for the speed dependence of line broadening and for Dicke narrowing, respectively. However, the results show that these effects have a negligible influence on the fit residuals and on the retrieved line-broadening coefficients. The pressure-broadening coefficients obtained from the rCMDS-calculated spectra at all considered temperatures are presented and compared with the experimental values in the next subsection.

3.2. H₂ broadening coefficient predicted by rCMDS

Figure 4 shows the broadening coefficients obtained from rCMDS at 296 K and their comparison with our accurate experimental values, where a very good agreement can be observed. Except for the P(2) line, for which a difference of 4% is observed, the discrepancies between the rCMDS predictions and the measured values are well below the experimental uncertainty (2%). We note that, for this comparison, the measured values were converted to 296 K using a single power law and the associated temperature dependence obtained from rCMDS, as listed in Appendix A. This level of agreement is significantly better than the precision of 10% required for opacity calculations in exoplanet studies with JWST (Wiesenfeld et al. 2025). In contrast, the current HITRAN data (red curve in Fig. 4, (Tan et al. 2022)) leads to substantial deviations of up to 16.5% relative to

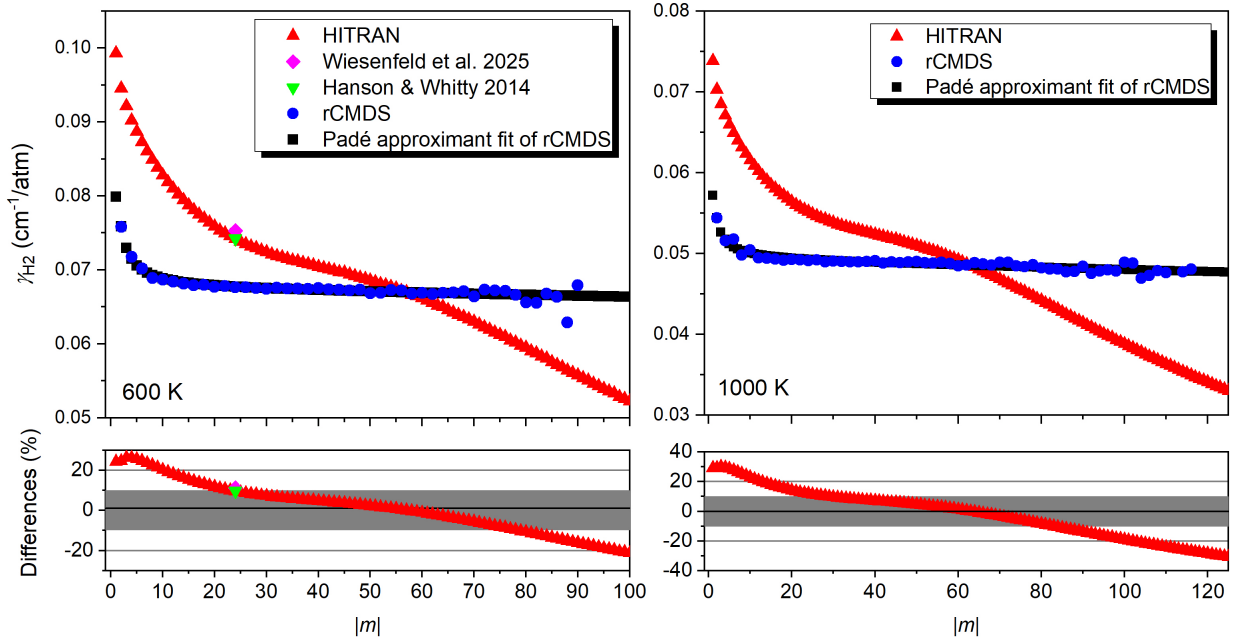


Fig. 5. H₂ broadening coefficient predicted by rCMDS at 600 K and 1000 K, and a comparison with values of HITRAN (Tan et al. 2022). The gray space represents the 10% precision level required for exoplanetary atmosphere studies.

the rCMDS values. The comparison presented in Fig. 4 therefore fully confirms the validity of our rCMDS method for predicting H₂ broadening coefficient of CO₂ lines.

rCMDS calculations were performed for six additional temperatures: 200 K, 400 K, 500 K, 600 K, 800 K, and 1000 K. For each temperature, γ_{H_2} was carefully determined for all considered lines. As the number of populated rotational levels increases with temperature, γ_{H_2} was determined up to a maximum rotational quantum number $J = 50$ at 200 K, while at 1000 K line broadening was obtained for lines up to $J = 120$. Figure 5 presents the rCMDS-predicted results at 600 K and 1000 K, together with corresponding γ_{H_2} values from HITRAN (Tan et al. 2022). Large discrepancies are observed at all temperatures, with deviations reaching more than 30%.

At 600 K, our results are also compared with the experimental measurements of Hanson & Whitty (2014), who measured the H₂ broadening coefficient for the P(24) line and provided a temperature dependence exponent of 0.582. The value calculated by Wiesenfeld et al. (2025) at 600 K for the same line is also shown. As illustrated in Fig. 5, our rCMDS results are about 10% smaller than those of Hanson & Whitty (2014) and Wiesenfeld et al. (2025). Nevertheless, given the excellent agreement between rCMDS predictions and accurate experimental data at room temperature (Fig. 4), as well as the improved validity of classical treatment for molecular rotations at higher temperatures, we are confident in the reliability of our results. Additional accurate measurements of H₂ broadening coefficients at temperatures above room temperature would nevertheless be valuable for further validation.

As can be seen in Figs. 4, 5, a noticeable scatter is present in the rCMDS-predicted broadening coefficients, particularly for high $|m|$ values. This scatter mainly arises from the lower signal-to-noise ratio of the corresponding lines, which leads to increased uncertainty in the extracted line broadening. To mitigate this effect, the rCMDS-predicted broadening coefficients at each temperature were fitted using a Padé approximant, as was done in Tan et al. (2022); Hendaoui et al. (2026). As illustrated

by the examples in Fig. 5, the quality of these fits is excellent. The fitted functions were then used to deduce broadening coefficients for R-branch lines, assuming symmetry between P- and R-branch coefficients with respect to m . This symmetry assumption has a negligible impact on the collisional line broadening of CO₂ (Mondelain et al. 2025). In addition, as γ_{H_2} tends toward a constant value at high J (see Figs. 4, 5), these functions can be safely used to extrapolate γ_{H_2} for J up to 120 for all considered temperatures. The fitted broadening coefficients were then used to determine their temperature dependence, which is presented in the following subsection.

3.3. Temperature dependence

We used both the usual single power law (SPL) and the recently recommended double power law (Gamache & Vispoel 2018) (DPL) to model the temperature dependence of γ_{H_2} . In the SPL, the temperature dependence of γ_{H_2} is expressed as

$$\gamma_{\text{H}_2}(T) = \gamma_{\text{H}_2}(T_0) \left(\frac{T_0}{T} \right)^n, \quad (2)$$

with $T_0 = 296$ K and n the temperature-dependence exponent. In the DPL, $\gamma_{\text{H}_2}(T)$ is written as

$$\gamma_{\text{H}_2}(T) = \gamma_0 \left(\frac{T_0}{T} \right)^{n_1} + \gamma'_0 \left(\frac{T_0}{T} \right)^{n_2}. \quad (3)$$

For each transition, both the SPL and DPL were fitted to the rCMDS-predicted values of γ_{H_2} at six temperatures: 200 K, 296 K, 400 K, 600 K, 800 K, and 1000 K. In the SPL fits the parameters $\gamma_{\text{H}_2}(T_0)$ and n were fitted, while in the DPL four parameters γ_0 , γ'_0 , n_1 and n_2 were fitted.

Figure 6 presents examples of fits with the SPL and DPL for the P(8) and R(28) lines. The corresponding differences between the rCMDS results and the fitted broadenings are also shown. As can be observed, the DPL provides better overall agreement with rCMDS predictions, with deviations always below 1%, whereas

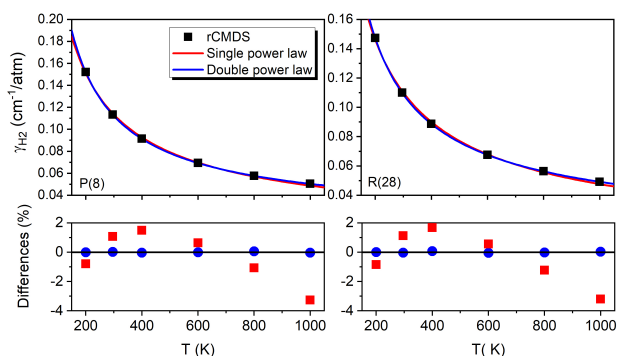


Fig. 6. rCMDS-predicted H_2 broadening coefficients vs. temperature (black squares) for two lines P(8) and R(28), and their fits using a single power function (red line) and a double power function (blue line). The differences between the rCMDS values and fits are displayed in the corresponding lower panels.

the SPL leads to discrepancies of up to 4%, especially at high temperatures.

Examples of the fitted parameters ($\gamma_{H_2}(T_0)$, n , γ_0 , γ'_0 , n_1 , and n_2), together with their standard deviations are reported in Appendix A, while the results for all considered lines are available on the Zenodo platform at the following link: <https://zenodo.org/records/18350127>. To further verify the quality of the fits, we recalculated γ_{H_2} using both the SPL and DPL parameterizations and compared the results with direct rCMDS predictions at 500 K. The results show very good agreement, with maximum deviations of 3% for the SPL and 1% for the DPL.

4. Conclusions

Accurate and comprehensive H_2 broadening coefficients for CO_2 lines under a wide temperature range are necessary for reliable opacity modeling of exoplanetary atmospheres. In this work, we reported the first accurate measurements at room temperature of H_2 broadening and pressure-shift coefficients for the entire CO_2 band at 4.3 μm , obtained using a high-resolution Fourier transform spectrometer. The commonly used data derived from air-broadening coefficients scaled by a constant factor show significant discrepancies, up to 16.5%, compared to the measured coefficients.

In addition, we performed first-principle calculations based on requantized classical molecular dynamics simulations (rCMDSs) to predict H_2 broadening coefficients of CO_2 lines over a wide temperature range, from 200 K to 1000 K. The predicted values are in very good agreement with the experimental measurements; the maximum differences are well below 3%, thus satisfying the precision requirements for JWST exoplanet studies. The experimentally validated rCMDS results were then used to derive the temperature dependence of the line broadening.

The obtained dataset allows the calculations of H_2 broadening coefficients for CO_2 lines with rotational quantum number up to 120 at any temperature within the 200–1000 K range. These results are expected to significantly improve the accuracy of opacity calculation for H_2 -rich atmosphere exoplanets.

Data availability

The complete dataset produced in this work are accessible at the following Zenodo link: <https://zenodo.org/records/18350127>.

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Appendix A: Additional table

Table A.1. Sample of parameters obtained from fits of the single power and double power laws to rCMDS results.

m	γ_{H_2}	n	γ_0	n_1	γ'_0	n_2
1	0.1382 (12)	0.761 (19)	0.1225 (25)	0.641 (112)	0.0130 (229)	2.204 (1549)
2	0.1280 (6)	0.728 (10)	0.1248 (28)	0.782 (22)	0.0024 (27)	-0.785 (615)
3	0.1221 (7)	0.719 (11)	0.1178 (7)	0.786 (5)	0.0034 (7)	-0.641 (108)
4	0.1191 (7)	0.713 (12)	0.1122 (12)	0.801 (8)	0.0059 (12)	-0.383 (96)
5	0.1173 (7)	0.709 (12)	0.1063 (23)	0.822 (13)	0.0098 (23)	-0.169 (95)
6	0.1160 (7)	0.706 (12)	0.1009 (35)	0.843 (18)	0.0140 (35)	-0.037 (93)
7	0.1152 (7)	0.704 (12)	0.0961 (41)	0.861 (20)	0.0179 (41)	0.050 (80)
8	0.1145 (7)	0.702 (12)	0.0912 (53)	0.881 (25)	0.0221 (53)	0.120 (79)
9	0.1140 (7)	0.701 (12)	0.0862 (66)	0.902 (31)	0.0266 (66)	0.178 (78)
10	0.1136 (7)	0.700 (13)	0.0832 (67)	0.914 (31)	0.0292 (66)	0.205 (71)
11	0.1133 (7)	0.699 (13)	0.0790 (75)	0.933 (36)	0.0331 (75)	0.243 (69)
12	0.1130 (7)	0.699 (13)	0.0770 (72)	0.942 (35)	0.0347 (72)	0.257 (63)
13	0.1127 (7)	0.698 (13)	0.0744 (69)	0.954 (35)	0.0371 (69)	0.276 (56)
14	0.1125 (7)	0.698 (13)	0.0734 (60)	0.958 (30)	0.0379 (60)	0.283 (47)
15	0.1124 (7)	0.698(13)	0.0718(58)	0.966 (30)	0.0393 (58)	0.294 (44)
16	0.1122 (7)	0.697 (13)	0.0697 (54)	0.976 (29)	0.0413 (54)	0.308 (39)
17	0.1121 (7)	0.697 (13)	0.0680 (45)	0.985 (24)	0.0429 (45)	0.319 (31)
18	0.1120 (7)	0.697 (13)	0.0678 (26)	0.986 (14)	0.0429 (26)	0.319 (18)
19	0.1118 (7)	0.697 (13)	0.0676 (27)	0.987 (14)	0.0429 (27)	0.319 (18)
20	0.1117 (7)	0.697 (13)	0.0676 (23)	0.986 (13)	0.0429 (23)	0.319 (16)
21	0.1117 (7)	0.697 (13)	0.0667 (28)	0.991 (15)	0.0437 (28)	0.325 (19)
22	0.1116 (7)	0.697 (13)	0.0681 (42)	0.984 (23)	0.0422 (42)	0.314 (30)
23	0.1115 (7)	0.697 (13)	0.0667 (49)	0.990 (27)	0.0435 (49)	0.324 (33)
24	0.1114 (7)	0.697 (13)	0.0667 (66)	0.991 (36)	0.0435 (66)	0.323 (45)
25	0.1114 (7)	0.697 (13)	0.0672 (78)	0.988 (42)	0.0429 (77)	0.319 (54)
26	0.1113 (7)	0.697 (13)	0.0673 (89)	0.987 (48)	0.0427 (88)	0.318 (62)
27	0.1112 (7)	0.697 (13)	0.0679 (99)	0.984 (54)	0.0420 (99)	0.313 (70)
28	0.1112 (7)	0.697 (13)	0.0682 (106)	0.982 (57)	0.0417 (106)	0.311 (76)
29	0.1111 (7)	0.697 (13)	0.0685 (125)	0.981 (67)	0.0414 (124)	0.309 (90)
30	0.1111 (7)	0.697 (13)	0.0698 (138)	0.974 (73)	0.0400 (138)	0.299 (103)
31	0.1110 (7)	0.697 (13)	0.0701 (143)	0.972 (76)	0.0397 (143)	0.296 (108)
32	0.1110 (7)	0.697 (13)	0.0706 (168)	0.970 (89)	0.0391 (168)	0.292 (129)
33	0.1110 (7)	0.697 (13)	0.0703 (178)	0.972 (94)	0.0394 (177)	0.295 (135)
34	0.1109 (7)	0.697 (13)	0.0716 (187)	0.964 (97)	0.0380 (186)	0.284 (148)
35	0.1109 (7)	0.697 (13)	0.0715 (203)	0.965 (106)	0.0381 (203)	0.285 (160)
36	0.1109 (7)	0.698 (13)	0.0725 (211)	0.960 (109)	0.0371 (210)	0.277 (172)
37	0.1108 (7)	0.698 (13)	0.0734 (230)	0.955 (119)	0.0362 (230)	0.269 (193)
38	0.1108 (7)	0.698 (13)	0.0728 (237)	0.959 (123)	0.0367 (236)	0.274 (195)
39	0.1108 (7)	0.698 (13)	0.0748 (246)	0.949 (126)	0.0348 (246)	0.257 (216)
40	0.1107 (7)	0.698 (13)	0.0752 (255)	0.946 (130)	0.0343 (255)	0.253 (227)
41	0.1107 (7)	0.698 (13)	0.0757 (273)	0.944 (138)	0.0338 (272)	0.249 (247)
42	0.1107 (7)	0.698 (13)	0.0761 (282)	0.942 (142)	0.0333 (281)	0.245 (259)
43	0.1107 (7)	0.698 (13)	0.0765 (290)	0.940 (146)	0.0329 (289)	0.241 (271)
44	0.1106 (7)	0.699 (13)	0.0765 (299)	0.940 (151)	0.0328 (298)	0.241 (280)
45	0.1106 (7)	0.699 (13)	0.0775 (312)	0.935 (156)	0.0319 (311)	0.232 (302)
46	0.1106 (7)	0.699 (13)	0.0783 (311)	0.931 (156)	0.0310 (310)	0.223 (312)
47	0.1106 (7)	0.699 (13)	0.0796 (318)	0.925 (158)	0.0297 (317)	0.211 (334)
48	0.1105 (7)	0.699 (13)	0.0796 (326)	0.925 (162)	0.0297 (325)	0.210 (344)
49	0.1105 (7)	0.699 (13)	0.0809 (328)	0.919 (162)	0.0284 (327)	0.196 (364)
50	0.1105 (7)	0.699 (13)	0.0809 (346)	0.919 (171)	0.0284 (345)	0.196 (385)
51	0.1105 (7)	0.700 (13)	0.0817 (351)	0.914 (174)	0.0275 (350)	0.187 (406)
52	0.1105 (7)	0.700 (13)	0.0821 (354)	0.913 (175)	0.0271 (352)	0.181 (416)

Notes. γ_{H_2} , γ_0 and γ'_0 are expressed in $\text{cm}^{-1}/\text{atm}$, while n , n_1 and n_2 are dimensionless.