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CO_2 pressure broadening and shift coefficients for the 1–0 band of HCl and DCl ☆

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ABSTRACT

CO_2 broadened spectra of the 1–0 band of $H^{35}Cl$ and $H^{37}Cl$, observed near 2886 cm^{-1}, and the 1–0 band of $D^{35}Cl$ and $D^{37}Cl$, located near 2089 cm^{-1}, have been recorded at room temperature and five total pressures between 150 and 700 Torr, using a Bruker IFS125HR Fourier transform spectrometer. Spectra of pure HCl were also recorded. CO_2 broadening and shift coefficients of HCl and DCl have been measured using multi-spectrum non-linear least squares fitting of Voigt profiles. The analysis of the 1–0 band of DCl was complicated by the presence of overlapping CO_2 bands, which were included in the treatment as absorption coefficients calculated taking line-mixing effects into account.

1. Introduction

Hydrogen chloride was discovered in the atmosphere of Venus in 1967 [1]. Using the Solar Occultation InfraRed (SOIR) high-resolution spectrometer [2] onboard the ESA Venus Express spacecraft, the vertical distribution of HCl in the Venus mesosphere (altitudes between 60 and 100 km) was measured for the first time [3]. Retrievals of hydrogen chloride by SOIR rely on a series of R branch lines of the 1–0 band, observed in the 2905–2995 cm^{-1} spectral range.

As the atmosphere of Venus is predominantly composed of carbon dioxide [4], knowledge of CO_2 broadening and shift coefficients of the HCl lines is required to retrieve hydrogen chloride concentrations from SOIR spectra. Measurements of CO_2 broadening coefficients of HCl lines have been reported more than 25 years ago [5–9]. Actually, retrievals of HCl from SOIR spectra [10] rely on CO_2 broadening coefficients reported by Toth and Darnton [8]. CO_2 shift coefficients appear to have been measured for the 2–0 band only [11,12]. Up to now, retrievals of hydrogen chloride from SOIR spectra approximated CO_2 shift with the air shift coefficients measured for the 1–0 band of $H^{35}Cl$ by Pine and Looney [13], reported in the HITRAN database [14].

In the context of SOIR measurements in the Venus mesosphere, the present work aimed to improve the available CO_2 broadening coefficients, and provide for the first time CO_2 pressure shift parameters for the 1–0 band of HCl. Although the temperature in the Venus mesosphere varies from about 170 to 270 K for altitudes in the range 60–160 km [15,16], the temperature dependence of these coefficients was not measured in the present work because it is believed to have a limited impact on the HCl retrievals from SOIR spectra. In addition, the same measurements were carried out for the 1–0 band of DCl, located near 2089 cm^{-1}. To the best of our knowledge, only the CO_2 broadening coefficient of R(1) of the 1–0 band of DCl was reported [5,17]. Note that the present measurements may also prove useful for future missions to Mars [18].

2. Experimental details

Unapodized room-temperature (296 K) absorption spectra of the 1–0 band of pure HCl at low pressure, and of HCl

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☆ This article is dedicated to Prof. Alain Barbe, Dr Claude Camy-Peyret and Dr Jean-Marie Flaud for their many contributions to science.

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or DCl mixed with CO_2 at five different total pressures between 150 and 700 Torr were recorded using a Bruker IFS 125 HR Fourier transform spectrometer. The instrument was fitted with a Tungsten source, an entrance aperture diameter of 0.8 mm (HCl) or 1.15 mm (DCl), a CaF_2 beamsplitter, a band-pass filter and a 77 K InSb detector. The band-pass filter had cut-off wavenumbers of about 2550–3150 cm^{-1} for HCl and about 1850–3450 cm^{-1} for DCl.

The HCl and DCl (99% stated purity) and CO_2 (99.8% stated purity) samples were purchased from Sigma–Aldrich. Pure HCl at low pressure, or mixtures of HCl or DCl with CO_2 were contained in a 21.1-cm long anodized aluminum cell, fitted with CaF_2 windows and located inside the evacuated spectrometer. The gas mixtures were prepared directly in the cell. Sample pressures were measured using two MKS Baratron gauges model 626, of 1000 and 10 Torr full-scale ranges.

Two series of experiments have been conducted for each isotopologue, leading to a total of 22 measurements. Each measurement involved the acquisition of 25 spectra, each corresponding to the average of two interferograms. Acquisition times for one spectrum ranged from 9.2 s to 4.8 min, from the lowest to the highest resolutions. The spectra were not averaged to account for the evolution of the HCl or DCl concentration during recording. These evolutions could result from the reactions of the acids with stainless steel pipes and valves connected to the cell, adsorption on the anodized aluminium cell walls, and/or DCl/HCl "conversion" as a result of the rapid deuterium–hydrogen exchange reactions; their exact origin was not investigated. Transmittances were generated for all the spectra using empty cell spectra recorded at the same instrumental conditions, except for the resolution set to 0.16 cm^{-1}. The total pressures, the HCl and DCl mole fractions, and the spectral resolutions used for each measurement are listed in Table 1. An example of the spectra recorded is presented in Fig. 1.

Table 1
Total pressure P_{tot}, initial x^i and final x^f mole fractions of HCl and DCl in the CO_2 mixtures, spectral resolution R (equal to 0.9 divided by the maximum optical path difference), and number of spectra considered in the analysis (n, 25 spectra were recorded in each measurement). The path length and temperature are, respectively, equal to 21.1(2) cm and 296(1) K for all the spectra.

#	P_{tot} (Torr)	x^i_{HCl} (%)	x^f_{HCl} (%)	x^i_{DCl} (%)	x^f_{DCl} (%)	R (cm^{-1})	n
1	0.1	1				0.005	20
2	150.2	0.252	0.148			0.02	25
3	300	0.276	0.222			0.04	25
4	451	0.291	0.256			0.06	25
5	600	0.291	0.271			0.08	9
6	700	0.301	0.285			0.1	9
7	0.1	1				0.002	25
8	150.2	0.308	0.219			0.02	25
9	300	0.243	0.208			0.04	25
10	450	0.252	0.229			0.06	25
11	600	0.259	0.243			0.08	9
12	700	0.267	0.255			0.1	9
13	150.0	0.388	0.600	0.820	0.308	0.01	23
14	301	0.348	0.575	0.890	0.516	0.02	25
15	453	0.205	0.450	1.020	0.710	0.03	23
16	601	0.221	0.400	1.000	0.794	0.04	22
17	700	0.192	0.300	1.100	0.934	0.05	22
18	150.7	0.541	0.640	0.650	0.289	0.01	23
19	301	0.432	0.630	0.775	0.444	0.02	25
20	450	0.319	0.520	0.910	0.629	0.03	23
21	601	0.254	0.400	1.000	0.788	0.04	22
22	700	0.192	0.320	1.100	0.908	0.05	22

The uncertainty on P_{tot} is equal to 0.5% of the value given, except for the pure HCl samples (spectra 1 and 7) for which the pressure is only approximate (see Section 3). The uncertainty on the mole fractions is equal to 1% of the value given.

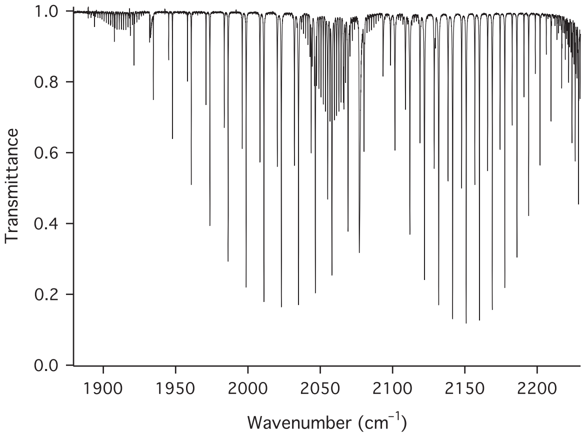

Fig. 1. Spectrum of the 1–0 band of $D^{35}Cl$ and $D^{37}Cl$ recorded in the present work (no. 22 in Table 1), corresponding to the average of two interferograms. Carbon dioxide absorption bands are observed around 1932, 2076 and above 2212 cm^{-1}.

3. Analysis

The line broadening and shift parameters were measured using a multi-spectrum least squares fitting algorithm, very recently developed in Brussels. We briefly present here the main aspects relevant to the present work.

The program adjusts a synthetic spectrum to each of any number of observed Fourier transform spectra, using a Levenberg–Marquardt least-squares fitting procedure. Each synthetic spectrum is calculated as the convolution of a monochromatic transmission spectrum with an instrument line shape function, which includes the effects of the finite maximum optical path difference and of the finite size of the entrance aperture in the interferometer [19]. In the present work, the background in each spectrum was represented by a constant, and the profile of the lines was modeled using a Voigt function [20], with Gaussian width always held fixed to the value calculated for the Doppler broadening. The pressure-induced widths b_L and shifts $\Delta\tilde{\nu}$ of the HCl and DCl lines were modeled according to:

$$b_L = P_{tot}[b_L^0(\mathrm{X{-}CO_2})(1-x) + b_L^0(\mathrm{self})x] \tag{1}$$

$$\Delta\tilde{\nu} = d^0(\mathrm{X{-}CO_2})P_{tot}(1-x) \tag{2}$$

where P_{tot} is the total sample pressure, x is the mole fraction of HCl or DCl, and $b_L^0(\mathrm{X{-}CO_2})$, $b_L^0(\mathrm{self})$ and $d^0(\mathrm{X{-}CO_2})$ are the CO_2-broadening, self-broadening, and CO_2-shift parameters of the HCl or DCl lines, respectively (X=HCl or DCl accordingly). Note that the notation

$b_L^0(X-Y)$ is used in the rest of the paper to identify the broadening coefficient of species X by species Y. As is apparent from Eq. (2), self-shift of hydrogen chloride and deuterium chloride lines was neglected as no such data is available for the 1–0 band.

The spectra of hydrogen chloride and deuterium chloride were analyzed separately. CO_2 pressure broadening and shift parameters of 1–0 band lines of the ^{35}Cl and ^{37}Cl isotopologues were retrieved from simultaneous fits of all the spectra usable for either HCl or DCl. The number of spectra included in the fits for each of the 22 experiments conducted is listed in Table 1. Each fit involved small spectral regions of about 5 cm^{-1}, in which P(J) or R(J) lines of both chlorine isotopologues corresponding to the same J are observed. The positions, intensities (including the isotopic abundances of H^{35}Cl and H^{37}Cl), and self-broadening parameters of the lines were held fixed to literature values (more details below). In addition to the CO_2 broadening and shift parameters of the HCl or DCl lines, all the measurements performed involved the adjustment of the mole fraction of the ^{35}Cl and ^{37}Cl isotopologues and a constant baseline for each spectrum included in the fit, and one calibration factor C applied to all the line positions according to $\tilde{\nu}_{calib} = \tilde{\nu}_{calc}(1+C)$, where $\tilde{\nu}_{calib}$ and $\tilde{\nu}_{calc}$ are the line positions calibrated and from the literature, respectively.

The mole fractions of HCl and DCl in the cell were thus measured for each spectrum treated. Their initial and final values for each measurement are listed in Table 1. In the HCl/CO_2 samples, a decrease with time of the HCl mole fraction was observed. When filling the cell, the mole fraction of DCl in the DCl/CO_2 samples was always set around 1%. Table 1 shows that "conversion" of DCl into HCl occurred in the cell as a result of the rapid deuterium–hydrogen exchange reactions. CO_2 broadening and shift coefficients were therefore also retrieved for HCl using the DCl/CO_2 spectra (thus identified as DCl/HCl/CO_2 from now on). In addition, because of the simultaneous presence of both species, mutual line shifting and broadening may affect the CO_2 broadening and shift parameters retrieved from these spectra. This point is discussed in Section 4.

3.1. Analysis of hydrogen chloride spectra

The positions, intensities, and self-broadening parameters of H^{35}Cl and H^{37}Cl lines were taken from the HITRAN database [14]. Note that the line positions therein were calculated using constants reported in [21], and the intensities and self-broadening parameters respectively originate from [22,23].

The fit of each P(J) or R(J) line of H^{35}Cl and H^{37}Cl involved the simultaneous adjustment (see Table 1) of 186 HCl/CO_2 spectra and 45 pure HCl spectra (for which the HCl mole fraction was obviously fixed to 1) or 230 DCl/HCl/CO_2 spectra. As an example, the result of the multispectrum fit of 231 observed spectra of the P(4) lines of H^{35}Cl and H^{37}Cl is presented in Fig. 2. This fit involved a total of 608 parameters [three parameters (constant baseline, and H^{35}Cl and H^{37}Cl mole fractions) for each HCl/CO_2 spectrum + one parameter (constant baseline) for each pure HCl spectrum + four line parameters (CO_2 broadening and shift coefficients for the H^{35}Cl and H^{37}Cl lines) + one calibration factor C], leading to an overall standard deviation equal to 6.6×10^{-3}. As can be seen, the standard Voigt profile appeared to fit appropriately the measured spectra to the noise level.

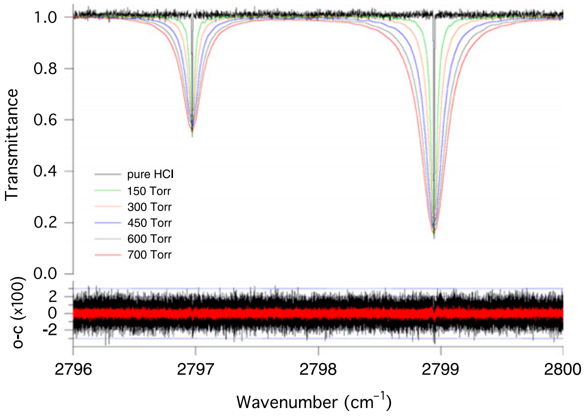

Fig. 2. Multi-spectrum fit of the P(4) lines of H^{35}Cl and H^{37}Cl. Six out of the 231 observed spectra fitted are shown in the upper panel, one for each pressure used in the fit (each spectrum is the average of two interferograms). The best-fit residuals for the 231 fitted spectra are presented in the lower panel, in black for the pure HCl spectra and in red for the others. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In the least squares fits just described, the total pressures of the 45 pure HCl spectra were held fixed. Because they were only measured approximately during recording, these HCl pressures were determined from a multi-spectrum fit of the 45 pure HCl spectra of the R(4) line of the 1–0 band only, using accurate (accuracy = 1–2% [14]) line intensities available [22]. That line was chosen because it is the strongest in the band. The HCl pressures thus obtained ranged from 0.03 to 0.05 Torr. We checked that the same pressures (within uncertainties) were obtained with two other strong lines, namely R(3) and P(6) of the 1–0 band. This method was chosen over the determination of the total pressures of the pure HCl spectra simultaneously with the CO_2 broadening and shift coefficients because the latter was found to lead to rather imprecise pure HCl pressures for weaker lines.

3.2. Analysis of deuterium chloride spectra

Transition energies of D^{35}Cl and D^{37}Cl were taken from [24], and the line intensities measured at 300 K by Benedict et al. [25] were converted to 296 K using Eq. 9 of [26]. Lower state energies required by the temperature conversion were calculated using the Dunham coefficients reported in [27] and the partition function was calculated at both temperatures using the product approximation, $Q = Q_v Q_r$ [28]. The vibrational partition function of deuterium chloride $Q_v = 1$ to better than 10^{-5} at 296 and 300 K. The rotational partition function Q_r was calculated according to McDowell [29], with the rotational constants reported in [27] to be 457.995 (464.142) and 459.334 (465.499) for D^{35}Cl and D^{37}Cl at 296 (300) K, respectively.

Self-broadening parameters of $D^{35}Cl$ and $D^{37}Cl$ lines in the 1–0 band were measured by Eaton and Thompson [17], for $m=1$–13 and 11, respectively (throughout the article, $m=-J''$, J'' and $J''+1$ for P-, Q- and R-branch lines, respectively). These measurements were fitted to the following expression:

$$b_L^0(\text{self}) = a_1 + a_2 m^2 + a_3 |m|^3 + a_4 m^4 \tag{3}$$

with standard deviations of 0.0091 and 0.011 $\text{cm}^{-1}\,\text{atm}^{-1}$ for $D^{35}Cl$ and $D^{37}Cl$, respectively. The best-fit coefficients are listed in Table 2. The self-broadening parameters of DCl lines were thus fixed to the values calculated using Eq. (3) and the coefficients in Table 2. Although the temperature of measurement is not mentioned in [17], it seems to be “room temperature”. We therefore assumed it to be the same as in the present measurements.

The fit of each P(J) or R(J) line of $D^{35}Cl$ and $D^{37}Cl$ proceeded in the same way as for hydrogen chloride, relying on 230 DCl/HCl/CO_2 observed spectra. As an example, the result of the multispectrum fit of the P(4) lines of $D^{35}Cl$ and $D^{37}Cl$ is shown in Fig. 3. This fit involved a total of 925 parameters, leading to an overall standard deviation equal to 2.2×10^{-3}. As can be seen, the standard Voigt profile also appeared to be appropriate to fit the measured spectra to the noise level.

As is apparent in Figs. 1 and 3, measurements for the 1–0 band of DCl were complicated by the presence of overlapping CO_2 absorption, possibly involving line-mixing when Q-branches were involved. To account for such contributions, we included in the modeling of the monochromatic spectrum, CO_2 absorbance spectra generated by a computer code written by Tran et al. [30]. A scaling factor multiplying the CO_2 absorbance was then adjusted to each observed spectrum, thus bringing to four the number of parameters fitted for each spectrum.

Table 2
Best-fit coefficients of Eq. (3) (× 1000) used to reproduce the measured self-broadening parameters of 1–0 band lines of deuterium chloride reported in [17].

	$D^{35}Cl$	$D^{37}Cl$
a_1	190.5(51)	187.2(71)
a_2	5.97(80)	5.4(14)
a_3	−1.11(14)	−0.94(30)
a_4	0.0477(67)	0.039(16)

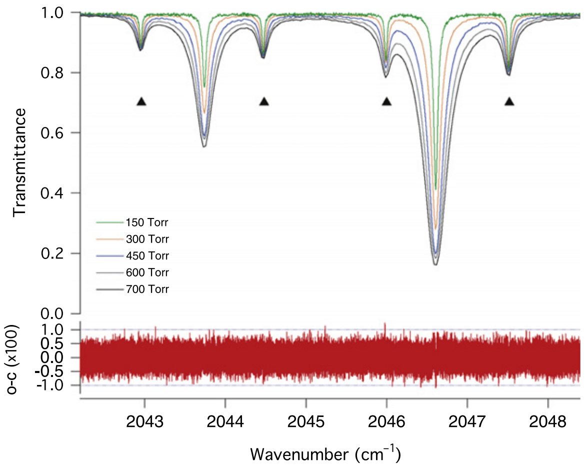

Fig. 3. Multi-spectrum fit of the P(4) lines of $D^{35}Cl$ and $D^{37}Cl$. Five out of the 230 observed spectra fitted are shown in the upper panel, one for each pressure used in the fit (each spectrum is the average of two interferograms). The best-fit residuals for the 230 fitted spectra are presented in the lower panel. The black triangles indicate CO_2 lines.

4. Results and discussion

4.1. CO_2 broadening parameters

The CO_2 pressure broadening coefficients measured in the present work for HCl and DCl are gathered in Tables 3 and 4 and Tables 7 and 8, respectively, and depicted in Fig. 4. These results show that the two sets of data measured for HCl agree well, despite the neglect of contributions from collisions with DCl in the DCl/HCl/CO_2 mixtures. Indeed, the CO_2 broadening coefficients of HCl retrieved from the DCl/HCl/CO_2 spectra are on average about 1% larger than those obtained from the HCl/CO_2 spectra [note that larger discrepancies are observed for some lines with $|m|\geq 9$, reaching 4% (9% for R(10) of $H^{37}Cl$)]. These observations tend to be confirmed by the rather limited contribution of DCl broadening of HCl lines in the DCl/HCl/CO_2 spectra. Indeed, using the total pressures, and initial and final HCl and DCl mole fractions listed in Table 1, and the b_L^0 (HCl–DCl) coefficients measured by James and Thibault [31], we estimated that DCl broadening of HCl lines represents at most 2% of the CO_2 broadening of the same lines in the DCl/HCl/CO_2 spectra. Similarly, the CO_2 broadening parameters obtained for DCl should also be affected by the presence of HCl. Applying the same procedure using the b_L^0 (DCl–HCl) coefficients also measured by James and Thibault [31], we estimated that HCl broadening of DCl lines represented less than 2% of the CO_2 broadening of the same lines.

Except for a few lines, differences between CO_2 pressure broadening coefficients obtained for the two chlorine isotologues are in the ranges 0.5–2% and 0.5–3% for DCl and the two sets of data measured for HCl, respectively, with averages around 1.5% and 2% (the ^{35}Cl broadening coefficients being larger). In contrast, b_L^0 (HCl–CO_2) and b_L^0 (DCl–CO_2) exhibit significant differences. Therefore the two data sets obtained for $H^{35}Cl$ and $H^{37}Cl$ on one hand and the data retrieved for $D^{35}Cl$ and $D^{37}Cl$ on the other hand were fitted separately to the following expression (inspired from [32]):

$$b_L^0 = a_1 m + \exp\left\{a_2 + a_3|m| + a_4 m^2 + a_5 m^4 + \frac{a_6}{|m|}\right\} \tag{4}$$

The best-fit coefficients and the corresponding overall standard deviations obtained are listed in Table 9. The broadening coefficients calculated using these coefficients and Eq. (4), and the corresponding residuals are also given in Tables 3, 4, 7, and 8 and Fig. 4.

Considering the discrepancies detailed here above, we estimated that the accuracy of the present CO_2 broadening coefficients is better than 3% for $|m|\leq 9$ and better

Table 3
CO$_2$ broadening parameters for the 1–0 band of H^{35}Cl at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	b_L^0 (H^{35}Cl–CO$_2$) (cm^{-1} atm^{-1})				
		Obs$_1$ (unc)	Obs$_2$ (unc)	Calc.	(O–C)$_1$	(O–C)$_2$
P(11)	2625.7256	0.0330(41)	0.0344(21)	0.03768	−14.	−9.5
P(10)	2651.9669	0.0370(26)	0.0379(23)	0.03974	−7.4	−4.8
P(9)	2677.7320	0.0414(14)	0.0424(13)	0.04298	−3.8	−1.5
P(8)	2703.0074	0.0472(15)	0.0478(14)	0.04764	−0.84	0.32
P(7)	2727.7795	0.0538(16)	0.0546(16)	0.05408	−0.44	0.90
P(6)	2752.0350	0.0625(19)	0.0634(19)	0.06283	−0.50	0.83
P(5)	2775.7605	0.0742(22)	0.0755(23)	0.07464	−0.54	1.1
P(4)	2798.9427	0.0895(27)	0.0909(27)	0.09049	−1.1	0.48
P(3)	2821.5684	0.1118(34)	0.1135(34)	0.1115	0.31	1.8
P(2)	2843.6245	0.1386(42)	0.1403(42)	0.1377	0.67	1.9
P(1)	2865.0981	0.1586(48)	0.1598(48)	0.1597	−0.67	0.09
R(0)	2906.2467	0.1587(48)	0.1600(48)	0.1599	−0.74	0.08
R(1)	2925.8965	0.1375(41)	0.1394(42)	0.1381	−0.45	0.92
R(2)	2944.9134	0.1098(33)	0.1117(34)	0.1121	−2.1	−0.38
R(3)	2963.2853	0.0891(27)	0.0908(27)	0.09138	−2.5	−0.62
R(4)	2981.0002	0.0751(23)	0.0765(23)	0.07576	−0.89	0.93
R(5)	2998.0464	0.0644(19)	0.0654(20)	0.06417	0.40	1.9
R(6)	3014.4123	0.0565(17)	0.0573(17)	0.05564	1.5	2.8
R(7)	3030.0866	0.0503(15)	0.0507(15)	0.04943	1.7	2.6
R(8)	3045.0582	0.0453(14)	0.0454(14)	0.04500	0.69	0.85
R(9)	3059.3162	0.0417(26)	0.0409(25)	0.04198	−0.67	−2.6
R(10)	3072.8500	0.0382(29)	0.0380(24)	0.04014	−5.0	−5.7
R(11)	3085.6493		0.0358(27)	0.03933		−9.8

The line positions $\tilde{\nu}$ are from [14]; the indices "1" and "2" identify measurements made in HCl/CO$_2$ and DCl/HCl/CO$_2$ samples, respectively; "unc" are the square root of the sum of the square of the estimated accuracy and the square of the statistical uncertainty (3σ) estimated by the least squares fit; the residuals (O–C) are expressed as a percentage of the corresponding observed value; the calculated values were obtained using Eq. (4) and the parameters listed in Table 9.

Table 4
CO$_2$ broadening parameters for the 1–0 band of H^{37}Cl at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	b_L^0 (H^{37}Cl–CO$_2$) (cm^{-1} atm^{-1})				
		Obs$_1$ (unc)	Obs$_2$ (unc)	Calc.	(O–C)$_1$	(O–C)$_2$
P(11)	2624.0314	0.0333(110)	0.0344(22)	0.03768	−13.	−9.5
P(10)	2650.2298	0.0380(45)	0.0375(23)	0.03974	−4.5	−6.1
P(9)	2675.9530	0.0408(23)	0.0423(13)	0.04298	−5.4	−1.7
P(8)	2701.1874	0.0477(18)	0.0475(14)	0.04764	0.17	−0.27
P(7)	2725.9197	0.0536(17)	0.0539(16)	0.05408	−0.91	−0.39
P(6)	2750.1364	0.0617(19)	0.0624(19)	0.06283	−1.9	−0.71
P(5)	2773.8242	0.0731(22)	0.0739(22)	0.07464	−2.1	−1.0
P(4)	2796.9699	0.0879(27)	0.0887(27)	0.09049	−3.0	−2.1
P(3)	2819.5603	0.1100(33)	0.1109(33)	0.1115	−1.3	−0.50
P(2)	2841.5825	0.1369(41)	0.1377(41)	0.1377	−0.56	0.03
P(1)	2863.0234	0.1567(48)	0.1576(47)	0.1597	−1.9	−1.3
R(0)	2904.1106	0.1564(48)	0.1574(47)	0.1599	−2.2	−1.6
R(1)	2923.7318	0.1356(41)	0.1365(41)	0.1381	−1.9	−1.2
R(2)	2942.7216	0.1079(33)	0.1090(33)	0.1121	−3.9	−2.9
R(3)	2961.0679	0.0874(26)	0.0884(27)	0.09138	−4.6	−3.4
R(4)	2978.7587	0.0738(22)	0.0746(22)	0.07576	−2.6	−1.5
R(5)	2995.7823	0.0636(19)	0.0642(19)	0.06417	−0.95	0.07
R(6)	3012.1272	0.0561(17)	0.0563(17)	0.05564	0.78	1.2
R(7)	3027.7822	0.0495(16)	0.0500(15)	0.04943	0.11	1.2
R(8)	3042.7361	0.0448(17)	0.0448(14)	0.04500	−0.48	−0.37
R(9)	3056.9781	0.0397(32)	0.0400(25)	0.04198	−5.7	−5.0
R(10)	3070.4976	0.0377(56)	0.0341(27)	0.04014	−6.6	−18.

The line positions $\tilde{\nu}$ are from [14]; the indices "1" and "2" identify measurements made in HCl/CO$_2$ and DCl/HCl/CO$_2$ samples, respectively; "unc" are the square root of the sum of the square of the estimated accuracy and the square of the statistical uncertainty (3σ) estimated by the least squares fit; the residuals (O–C) are expressed as a percentage of the corresponding observed value; the calculated values were obtained using Eq. (4) with the parameters listed in Table 9.

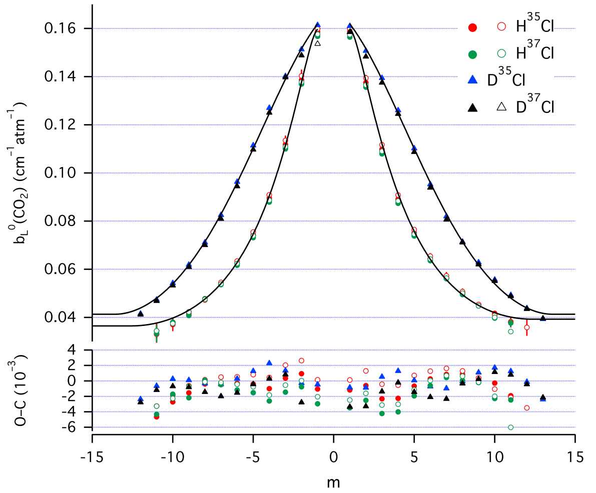

Fig. 4. CO_2 broadening parameters for the 1–0 band of HCl and DCl. Upper panel: measurements (for HCl, filled and open circles correspond to HCl/CO_2 and $DCl/HCl/CO_2$ spectra, respectively; for DCl, the open triangle identifies a data point excluded from the fit to Eq. (4)), and calculated values using Eq. (4) and the coefficients in Table 9 (solid curves). Lower panel: corresponding residuals. Error bars represent the uncertainties (1σ) estimated by the least squares fitting algorithm.

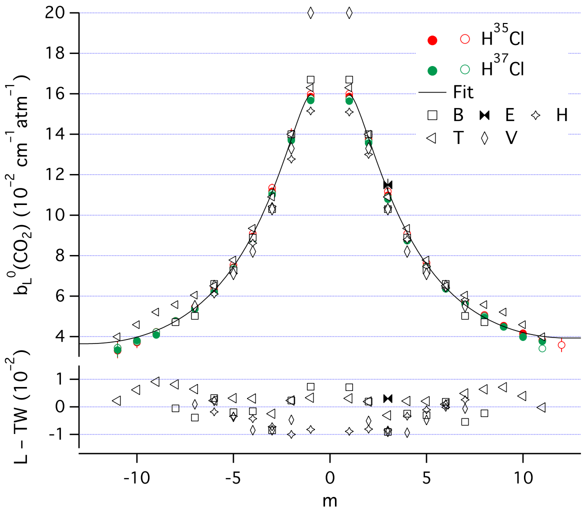

Fig. 5. Comparison of CO_2 broadening coefficients measured for the 1–0 band of HCl in this and previous work. The filled and open circles (see legend of Fig. 4), and curves are from this work, and "B", "E", "H", "T" and "V" refer to [6,5,9,8,7], respectively. The differences between values from the literature ("L") and calculated in this work ("TW", using Eq. (4) and the coefficients in Table 9) are shown in the lower panel (the two values at $|m|=1$ from [7] are off-scale).

than 6% for larger m. To account for measurement errors, the uncertainties given in the tables are set to the square root of the sum of the square of these limiting accuracies and the square of the statistical uncertainties (3σ) estimated by the least squares fitting procedure (1σ ranging from 0.1% for low to intermediate m, to a few % for $m\approx 10$). The latter statistical uncertainties are shown as 1σ error bars in Fig. 4. Note that the CO_2 broadening coefficients of HCl lines retrieved from the $DCl/HCl/CO_2$ spectra seemed to be slightly more precise than those obtained from the HCl/CO_2 spectra, probably because the HCl mole fraction turned out to be larger in the former (especially at the lower total pressures, see Table 1).

As already indicated, CO_2 broadening coefficients have already been measured for the 1–0 band of HCl at room temperature (295–300 K) [5–9]. Although these previous measurements were carried out at pressures (≥ 1 atm) higher than in the present work (except for [5]), Fig. 5 shows that they agree well with the present values. In particular, our results agree very well with the Toth and Darnton [8] measurements in the spectral range probed by the SOIR spectrometer ($m=1$–5). The most important discrepancies are observed with Varanasi et al. [7] for $|m|=1$. Note that Varanasi et al. [7] reported measurements up to $|m|=12$ only in a figure (Fig. 1); the numerical values given in Fig. 5 were taken from Table I of [9]. The values for $|m|>7$ in Fig. 1 of [7] seem to agree with the present results.

For DCl, it seems that only the CO_2 broadening coefficient of the R(1) line of the 1–0 band was measured. Indeed, Eaton and Thompson reported two measurements most probably at "room temperature": 0.147 cm^{-1} atm^{-1} [5] and 0.0927 cm^{-1} atm^{-1} [17]. These values exhibit discrepancies of -1.7 and -38% with the average of the present measurements for D^{35}Cl and D^{37}Cl, i.e. b_L^0 (DCl–CO_2)=0.1496(45) cm^{-1} atm^{-1}.

The introduction of an asymmetry between the P and R branches (a_1 in Eq. (4)) resulted in a better fit of the CO_2 broadening parameters measured for HCl (see Fig. 4). The CO_2 broadening parameters reported for the same band by Houdeau et al. [9] also exhibit such a small P/R asymmetry. In the present work, the fit of the DCl data could also be very marginally improved in the same way (a_1 could be determined, but was only slightly larger than the 1σ estimated uncertainty). Considering the spread of our measurements in Fig. 4, it is clear that this observation deserves confirmation.

4.2. CO_2 shift parameters

The CO_2 shift coefficients of HCl and DCl measured in the present work are gathered in Tables 5–8 and depicted in Fig. 6. To the best of our knowledge, this is the first experimental determination of these parameters for the 1–0 band. The uncertainties of measurement (estimated by the least squares fitting algorithm) are slightly larger for P(6) to R(3) for DCl compared to results obtained for other lines, mainly because these lines are overlapped by CO_2 absorption.

Pressure-induced self shift coefficients have been measured for the 2–0 band of H^{35}Cl and H^{37}Cl at a series of pressures in the range from 50 to 700 Torr [33] and at 10 Torr [12]. Pressure-induced shift coefficients of HCl by DCl and DCl by HCl have also been reported for 2–0 band lines [34,35]. Assuming that pressure-induced shifts are proportional to band centers [36,37] and relying on the total pressures, and initial and final HCl and DCl mole fractions listed in Table 1, these reported values were used to (roughly)

Table 5
CO_2 shift parameters for the 1–0 band of $H^{35}Cl$ at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	d^0 ($H^{35}Cl$–CO_2) ($\times 10^4$ cm^{-1} atm^{-1})			
		Obs$_1$	U (%)	Obs$_2$	U (%)
P(11)	2625.7256	−152.	3.9	−149.	0.66
P(10)	2651.9669	−137.	1.8	−145.	0.32
P(9)	2677.7320	−129.	1.0	−130.	0.21
P(8)	2703.0074	−107.	0.75	−111.	0.17
P(7)	2727.7795	−81.6	0.72	−85.1	0.19
P(6)	2752.0350	−54.8	0.93	−57.4	0.28
P(5)	2775.7605	−30.5	1.6	−34.4	0.52
P(4)	2798.9427	−16.8	2.91	−20.2	1.0
P(3)	2821.5684	−55.7	0.97	−58.2	0.45
P(2)	2843.6245	−81.5	0.79	−83.4	0.42
P(1)	2865.0981	−83.3	1.2	−87.9	0.60
R(0)	2906.2467	48.5	1.9	49.1	1.2
R(1)	2925.8965	39.2	1.5	38.1	1.2
R(2)	2944.9134	−8.82	5.4	−11.4	3.4
R(3)	2963.2853	−69.3	0.62	−74.0	0.50
R(4)	2981.0002	−86.5	0.46	−91.9	0.38
R(5)	2998.0464	−114.	0.35	−120.	0.29
R(6)	3014.4123	−140.	0.30	−145.	0.26
R(7)	3030.0866	−160.	0.33	−165.	0.27
R(8)	3045.0582	−179.	0.46	−180.	0.35
R(9)	3059.3162	−187.	0.86	−192.	0.57
R(10)	3072.8500	−200.	1.9	−208.	1.2
R(11)	3085.6493			−213.	2.9

The line positions $\tilde{\nu}$ are from [14]; the indices "1" and "2" indicate measurements made in HCl/CO_2 and $DCl/HCl/CO_2$ samples, respectively; the estimated statistical uncertainties U (1σ) are expressed as a percentage of the corresponding observed value.

Table 6
CO_2 shift parameters for the 1–0 band of $H^{37}Cl$ at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	d^0 ($H^{37}Cl$–CO_2) ($\times 10^4$ cm^{-1} atm^{-1})			
		Obs$_1$	U (%)	Obs$_2$	U (%)
P(11)	2624.0314	−123.	15.	−142.	1.2
P(10)	2650.2298	−147.	5.4	−140.	0.56
P(9)	2675.9530	−123.	2.8	−125.	0.34
P(8)	2701.1874	−105.	2.0	−106.	0.26
P(7)	2725.9197	−79.7	1.6	−81.2	0.27
P(6)	2750.1364	−51.5	1.9	−52.7	0.40
P(5)	2773.8242	−27.2	3.1	−29.5	0.75
P(4)	2796.9699	−12.2	6.8	−15.0	1.7
P(3)	2819.5603	−51.1	1.9	−53.1	0.60
P(2)	2841.5825	−76.9	1.7	−78.2	0.59
P(1)	2863.0234	−76.8	3.1	−79.2	0.96
R(0)	2904.1106	49.3	4.5	49.0	1.7
R(1)	2923.7318	44.0	2.7	42.5	1.4
R(2)	2942.7216	−5.47	14.	−7.37	6.4
R(3)	2961.0679	−64.6	1.0	−68.6	0.63
R(4)	2978.7587	−82.0	0.74	−85.2	0.48
R(5)	2995.7823	−110.	0.60	−114.	0.37
R(6)	3012.1272	−134.	0.62	−139.	0.35
R(7)	3027.7822	−155.	0.71	−159.	0.39
R(8)	3042.7361	−175.	1.2	−175.	0.54
R(9)	3056.9781	−178.	2.1	−184.	0.98
R(10)	3070.4976	−190.	5.3	−205.	1.9
R(11)	3083.2844			−198.	5.0

The line positions $\tilde{\nu}$ are from [14]; the indices "1" and "2" indicate measurements made in HCl/CO_2 and $DCl/HCl/CO_2$ samples, respectively; the estimated statistical uncertainties U (1σ) are expressed as a percentage of the corresponding observed value.

estimate the corresponding contributions to the CO_2 shift coefficients obtained in the present work.

The CO_2 pressure-induced shift coefficients determined for the 1–0 band of $H^{35}Cl$ and $H^{37}Cl$ from the HCl/CO_2 spectra could include contributions from self shift. Relying on the coefficients reported by Guelachvili and Smith [12], we estimated that these contributions were smaller than 1% of the CO_2 shifts for the lines with $m < -5$ and $m > 3$ (characterized by larger pressure-induced shifts), and were in the range 1–2% for the remaining lines (except for the line at $m=3$ for which the very small CO_2 shift leads to a contribution of self shift of about 5%). Using the self shift coefficients reported by Kimel et al. [33], significantly smaller self shift contributions were estimated, being at most 1% of the CO_2 shifts for all the lines.

The CO_2 shift coefficients of HCl lines retrieved from the $DCl/HCl/CO_2$ spectra are on average 3–4% more negative than those obtained from the HCl/CO_2 spectra. In addition to self shift (which could contribute more to the CO_2 shifts because the HCl mole fractions were larger than in the HCl/CO_2 spectra), the CO_2 shift coefficients determined for HCl from the $DCl/HCl/CO_2$ spectra could contain contributions from shifts by DCl. Using the self [12] and HCl by DCl [34] shift coefficients available for the 2–0 band, we estimated that their combined contributions to the CO_2 shift coefficients of the 1–0 band of HCl measured in the $DCl/HCl/CO_2$ spectra were smaller than 1% of the CO_2 shifts for $m < -5$ and $m > 3$, and were in the range 1–3% for the remaining lines, reaching 10% for $m=3$. These contributions seem to only partially explain the observed discrepancies between the shift coefficients retrieved from the HCl/CO_2 and $DCl/HCl/CO_2$ spectra.

Similarly, the CO_2 shift coefficients determined for DCl could be affected by self shift and shift by HCl. Unfortunately, it was not possible to estimate the contribution from self shift as the corresponding coefficients do not seem to have ever been measured for DCl. Comparison between Fig. 1 of [35] and Fig. 6 shows that d^0 (DCl–HCl) and d^0 (DCl–CO_2) are roughly similar. As the mole fraction of HCl in the $DCl/HCl/CO_2$ samples was always less than 1%, the corresponding contributions to the CO_2 shifts of DCl can therefore be expected to be of the same magnitude.

The rather rough estimates detailed here above tend to indicate that contributions from "non-CO_2" pressure-induced shifts to the CO_2 shifts measured in this work are probably generally small, with the possible exception of a few lines characterized by small CO_2 shift coefficients. Because of this and the potentially large uncertainties associated with these estimates, the CO_2 shift parameters reported here were not corrected for these contributions.

As already mentioned, CO_2 pressure-induced shift coefficients have been measured for the 2–0 band of $H^{35}Cl$ and $H^{37}Cl$ [11,12]. These measurements are compared with the present work in Fig. 7. The three sets of data follow a similar rotational dependence and exhibit a rather good agreement, taking the vibrational dependence of the pressure-induced shift coefficients into account. The air shift coefficients measured for the 1–0 band of $H^{35}Cl$ by Pine and Looney [13] and used up to now in

Table 7
CO_2 broadening and shift parameters (cm^{-1} atm^{-1}) for the 1–0 band of D^{35}Cl at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	b_L^0 (D^{35}Cl–CO$_2$)			d^0 ($\times 10^4$)	
		Obs. (unc)	Calc.	O–C	Obs.	U (%)
P(12)	1947.7901	0.0416(25)	0.04393	−5.7	−72.1	0.50
P(11)	1960.8202	0.0474(28)	0.04803	−1.4	−55.6	0.50
P(10)	1973.6636	0.0542(33)	0.05397	0.47	−39.7	0.55
P(9)	1986.3171	0.0619(19)	0.06178	0.15	−23.5	0.85
P(8)	1998.7766	0.0711(21)	0.07146	−0.45	−16.2	1.2
P(7)	2011.0390	0.0825(25)	0.08294	−0.52	−12.9	1.6
P(6)	2023.1006	0.0963(29)	0.09598	0.30	−11.6	1.9
P(5)	2034.9579	0.1114(33)	0.1101	1.1	−15.5	1.5
P(4)	2046.6074	0.1270(38)	0.1247	1.8	−32.1	0.81
P(3)	2058.0457	0.1402(42)	0.1389	0.95	−31.7	1.0
P(2)	2069.2692	0.1513(45)	0.1516	−0.19	−33.8	1.1
P(1)	2080.2747	0.1614(48)	0.1619	−0.29	−98.6	0.62
R(0)	2101.6178	0.1610(48)	0.1619	−0.54	68.1	0.82
R(1)	2111.9488	0.1507(45)	0.1516	−0.59	4.29	7.7
R(2)	2122.0483	0.1394(42)	0.1389	0.38	−0.931	28.
R(3)	2131.9131	0.1260(38)	0.1247	1.0	−13.4	1.6
R(4)	2141.5398	0.1102(33)	0.1101	0.06	−38.5	0.52
R(5)	2150.9255	0.0953(29)	0.09598	−0.75	−52.2	0.35
R(6)	2160.0668	0.0820(25)	0.08294	−1.2	−69.8	0.24
R(7)	2168.9608	0.0714(21)	0.07146	−0.06	−90.9	0.18
R(8)	2177.6042	0.0629(19)	0.06178	1.7	−111.	0.14
R(9)	2185.9942	0.0557(33)	0.05397	3.1	−126.	0.14
R(10)	2194.1277	0.0493(30)	0.04803	2.5	−142.	0.14
R(11)	2202.0018	0.0438(26)	0.04393	−0.30	−153.	0.18
R(12)	2209.6136	0.0393(24)	0.04170	−6.1	−164.	0.20

The line positions $\tilde{\nu}$ are from [24]; the uncertainties "unc" provided for b_L^0 (D^{35}Cl–CO$_2$) are the square root of the sum of the square of the estimated accuracy and the square of the statistical uncertainty (3σ) estimated by the least squares fit; the calculated values were obtained using Eq. (4) and the parameters listed in Table 9; d^0 represents d^0 (D^{35}Cl–CO$_2$); the estimated statistical uncertainties U (1σ) provided for d^0 (D^{35}Cl–CO$_2$) are expressed as a percentage of the corresponding observed value.

Table 8
CO_2 broadening and shift parameters (cm^{-1} atm^{-1}) for the 1–0 band of D^{37}Cl at 296 K.

Line	$\tilde{\nu}$ (cm^{-1})	b_L^0 (D^{37}Cl–CO$_2$)			d^0 ($\times 10^4$)	
		Obs. (unc)	Calc.	O–C	Obs.	U (%)
P(12)	1945.2288	0.0412(25)	0.04393	−6.7	−70.1	1.4
P(11)	1958.2179	0.0469(28)	0.04803	−2.5	−54.4	0.79
P(10)	1971.0209	0.0533(32)	0.05397	−1.3	−37.6	0.88
P(9)	1983.6348	0.0610(18)	0.06178	−1.3	−22.4	1.3
P(8)	1996.0557	0.0700(21)	0.07146	−2.0	−14.5	1.8
P(7)	2008.2801	0.0809(24)	0.08294	−2.5	−12.1	2.1
P(6)	2020.3046	0.0944(28)	0.09598	−1.6	−9.67	2.8
P(5)	2032.1257	0.1097(33)	0.1101	−0.39	−13.6	2.1
P(4)	2043.7399	0.1250(38)	0.1247	0.22	−30.0	1.1
P(3)	2055.1438	0.1397(42)	0.1389	0.59	−24.2	1.9
P(2)	2066.3339	0.1488(45)	0.1516	−1.9	−29.3	1.9
P(1)	2077.3068	0.1536(47)	0.1619		−72.6	2.3
R(0)	2098.5878	0.1585(48)	0.1619	−2.1	75.8	1.2
R(1)	2108.8892	0.1483(45)	0.1516	−2.2	4.50	11.
R(2)	2118.9601	0.1375(41)	0.1389	−1.0	−0.0182	1900.
R(3)	2128.7975	0.1245(37)	0.1247	−0.18	−10.8	2.7
R(4)	2138.3978	0.1087(33)	0.1101	−1.3	−36.5	0.66
R(5)	2147.7581	0.0939(28)	0.09598	−2.2	−50.4	0.44
R(6)	2156.8752	0.0806(24)	0.08294	−2.9	−67.7	0.30
R(7)	2165.7460	0.0711(21)	0.07146	−0.47	−90.6	0.22
R(8)	2174.3675	0.0620(19)	0.06178	0.38	−109.	0.19
R(9)	2182.7367	0.0551(33)	0.05397	2.1	−123.	0.19
R(10)	2190.8505	0.0488(29)	0.04803	1.6	−140.	0.21
R(11)	2198.7062	0.0435(26)	0.04393	−1.0	−149.	0.29
R(12)	2206.3006	0.0395(24)	0.04170	−5.5	−161.	0.33

The line positions $\tilde{\nu}$ are from [24]; the uncertainties "unc" provided for b_L^0 (D^{37}Cl–CO$_2$) are the square root of the sum of the square of the estimated accuracy and the square of the statistical uncertainty (3σ) estimated by the least squares fit; the calculated values were obtained using Eq. (4) and the parameters listed in Table 9; d^0 represents d^0 (D^{37}Cl–CO$_2$); the estimated statistical uncertainties U (1σ) provided for d^0 (D^{37}Cl–CO$_2$) are expressed as a percentage of the corresponding observed value.

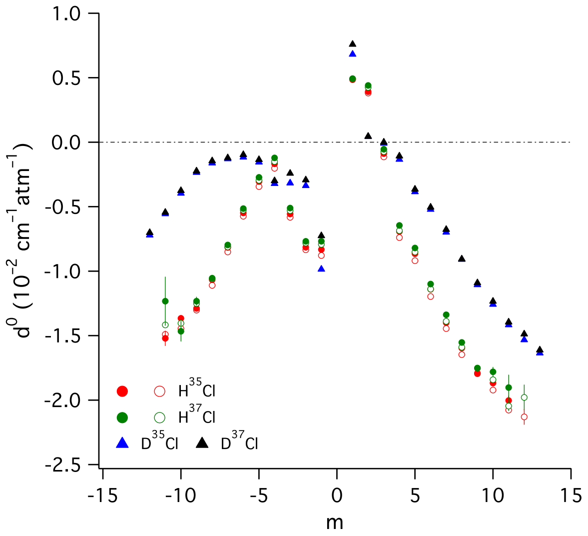

Fig. 6. CO_2 shift coefficients measured for the 1–0 band of HCl and DCl. For hydrogen chloride, the filled and open circles correspond to measurements in the HCl/CO_2 and $DCl/HCl/CO_2$ samples, respectively.

Table 9
Best-fit parameters of Eq. (4) ($\times 1000$) and corresponding overall standard deviations (in cm^{-1} atm^{-1}) that reproduce the CO_2 broadening parameters measured for the 1–0 band of hydrogen and deuterium chloride at 296 K.

	HCl	DCl
a_1	0.112(25)	0.
a_2	−1266.(22)	−1779.(12)
a_3	−317.0(65)	−30.5(61)
a_4	12.65(54)	−11.87(79)
a_5	0.	0.0352(29)
a_6	−264.(18)	0.
σ	1.2×10^{-3}	1.2×10^{-3}

Numbers between parentheses are the uncertainties (1σ) in the units of the last quoted digit. Values without uncertainties were held fixed to the values given.

retrievals of hydrogen chloride from SOIR spectra are also presented in Fig. 7. In the spectral range probed by SOIR, CO_2 shift coefficients are either in very good agreement with the air shifts ($m=4$–5) or of opposite sign ($m=2$).

In Fig. 8, the CO_2 shift coefficients are presented vs. the CO_2 broadening coefficients associated to the same line to investigate any correlations between them. For the R branch of both isotopologues, the shift coefficients become less negative with increasing broadening coefficients. A similar trend is observed for the P branch up to $b_L^0(CO_2) \approx 0.09$ cm^{-1} atm^{-1}, followed by the opposite trend for larger broadening coefficients. Interestingly, whereas the R branches of both isotopologues have apparently the same behavior, the evolution observed for the P branch of DCl is about 2.5 times smaller than for HCl.

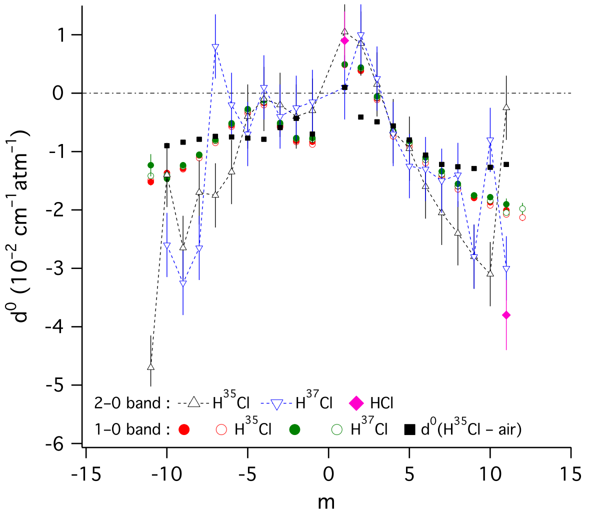

Fig. 7. Comparison of CO_2 shift coefficients measured for the 1–0 band (this work) and the 2–0 band (measurements from [12] and [11] are represented by open triangles and diamonds, respectively) of $H^{35}Cl$ and $H^{37}Cl$. For the 1–0 band, the filled and open circles correspond to measurements in the HCl/CO_2 and $DCl/HCl/CO_2$ samples, respectively. The black squares are the air shift coefficients measured for the 1–0 band of $H^{35}Cl$ [13].

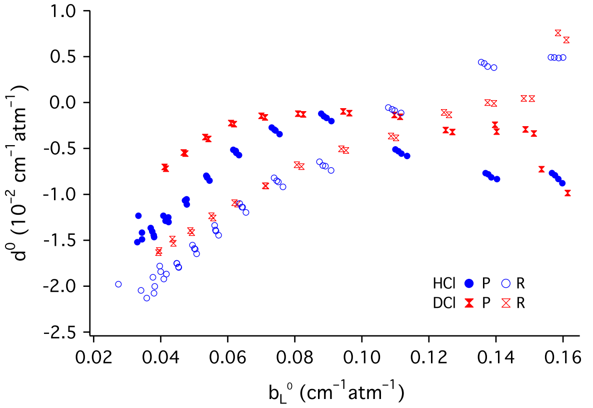

Fig. 8. CO_2 shift coefficients vs. the CO_2 broadening coefficients associated to the same line of the 1–0 band of HCl and DCl.

5. Conclusion

A global analysis of high-resolution Fourier transform spectra of HCl and DCl diluted in CO_2 at total pressures up to 700 Torr with a multispectrum least squares fitting technique resulted in the determination of CO_2 broadening and shift coefficients for 1–0 band lines of HCl and DCl, up to $J=11$. A Voigt function appeared to properly model the observed molecular line shapes within the noise level. The accuracy of the CO_2 broadening coefficients obtained for HCl and DCl was estimated to be better than 3% for $|m| \leq 9$ and better than 6% up to $m=12$. Not enough information was available to properly estimate the accuracy of the shift coefficients. The broadening parameters measured for HCl in this work are in good agreement with previous measurements, as do the CO_2 shift coefficients with earlier measurements for the 2–0 band.

Acknowledgments

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