I. Improvement for line position and line intensities

Accurate line positions, line intensities and Einstein $A$-coefficients were calculated for all possible ro-vibrational transitions (fundamental, overtone, and hot bands) for hydrogen halides, HF, HCl, HBr, HI and their deuterated isotopologues, up to the maximum $v, J$ levels that are listed in Table 1. Note that the deuterated isotopologues of these species appear in HITRAN for the first time. The calculation employs the recently developed semi-empirical dipole moment functions [1] and very accurate potential energy functions which include the parameters characterizing the Born-Oppenheimer breakdown effects [2]. In Table 1, the choice of the maximum $v, J$ levels for different molecules were mainly based on the highest ro-vibrational level that is measured experimentally in high resolution. For example, $v = 22, J = 80$ for $D^{35,37}Cl$ means the nearby $v, J$ level was measured experimentally for $D^{35,37}Cl$. The evaluation of the calculated line position and intensities can be found in the works by Li, Gordon, Le Roy, Hajigeorgiou, Coxon, Bernath, and Rothman [1, 3] in detail. Nevertheless, Fig. 1 shows an example of the huge improvements for line positions of HI compared with HITRAN2008.

![Graph showing comparison of line position with HITRAN 2008](image_url)

Figure 1: Comparison of the line position from the present study with HITRAN 2008 using G. Guelachvili’s experimental study [4] as a reference. The large deviation of HITRAN 2008 is due to extrapolation from the lower vibrational level.
Table 1. The maximum $\nu,J$ range of the calculation.

<table>
<thead>
<tr>
<th></th>
<th>$\nu_{\text{max}}$</th>
<th>$J_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1H^{19}F$</td>
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<td>40</td>
</tr>
<tr>
<td>$^3D^{19}F$</td>
<td>26</td>
<td>40</td>
</tr>
<tr>
<td>$H^{35,37}Cl$</td>
<td>17</td>
<td>40</td>
</tr>
<tr>
<td>$D^{35,37}Cl$</td>
<td>22</td>
<td>80</td>
</tr>
<tr>
<td>$H^{79,81}Br$</td>
<td>7</td>
<td>40</td>
</tr>
<tr>
<td>$D^{79,81}Br$</td>
<td>5</td>
<td>40</td>
</tr>
<tr>
<td>$H^{127}I$</td>
<td>7</td>
<td>40</td>
</tr>
<tr>
<td>$D^{127}I$</td>
<td>5</td>
<td>40</td>
</tr>
</tbody>
</table>

II. Revised hyperfine structure

HCl: The hyperfine structure (hfs) components for the $X^1\Sigma^+ 0-0$ $H^{35}Cl, H^{37}Cl$ bands were regenerated for $J \leq 15$ with improved ground state parameters from Cazzoli and Puzzarini [5]. The sum of the relative line intensities of the hfs components, calculated using the PGOPHER program [29], was normalized to the intensity of the corresponding rotational line from the study of Li et al. [1, 6]. Figure 2 shows the improvement in transition frequencies for the high-$J$ lines of the 0-0 band of $H^{35}Cl$.

![Figure 2: Comparison of the HITRAN2008, experimental [5], and the present calculated line positions of the 0-0 band of $H^{35}Cl$ with the present study as a reference. For lines with $J'' \leq 15$, hyperfine structure is resolved.](image-url)
DCl: New hyperfine structure components for the $X^1\Sigma^+\ 0-0\ D^{35}\text{Cl}, D^{37}\text{Cl}$ bands were calculated using the ground state parameters from Cazzoli and Puzzarini [7]. The sum of the relative line intensities of the hfs components, calculated with the PGOPHER program, was normalized to the intensity of the corresponding rotational line from the study by Li et al. [1, 6].

HBr: The line positions of the hfs components for the $X^1\Sigma^+\ (0-0)$ and (0-1) $H^{79}\text{Br}, H^{81}\text{Br}$ bands were retained from the HITRAN2008 listing. However, the high-$J$ rotational line positions without hfs structure of the same bands were recalculated using the semi-empirical potential from Coxon and Hajigeorgiou [2]. The sum of the relative line intensities of the hfs components, was normalized to the intensity of the corresponding rotational line from the study by Li et al. [1].

DBr: No hyperfine structure components were added.

HI: The line positions of the hfs components for the $X^1\Sigma^+\ (0-0)$ and (0-1) $H^{127}\text{I}$ bands were retained from the HITRAN2008 listing. The line positions of the high-$J$ rotational lines of the same bands were recalculated using the semi-empirical potential from Coxon and Hajigeorgiou [2]. The sum of the relative line intensities of the hfs components, was normalized to the intensity of the corresponding rotational line from the study by Li et al [1].

DI: The calculated line positions for the $X^1\Sigma^+\ 0-0\ D^{127}\text{I}$ bands including the hyperfine structure components were included from the work by Varberg et al. [8]. The line positions of the high-$J$ rotational lines of the same bands were recalculated using the semi-empirical potential from Coxon and Hajigeorgiou [2]. The sum of the relative line intensities of the hfs components, calculated using the PGOPHER program was normalized to the intensity of the corresponding rotational line from the study by Li et al. [1].

III. Line shape parameters

$\gamma_{air}$: For the fundamental band, the air-broadening parameters for HF in the HITRAN2008 compilation turned out to be fitted not with a Voigt profile, but with the Galatry profile based on the Pine and Looney [9] measurements. However, the Dicke narrowing parameter was not provided in the previous database. The corresponding collisional, or Dicke, narrowing parameters have been cast into a separate columnar table that is easily linked to the main part of HITRAN using the unique combination of: molecule number, isotopologue number, and quantum identifications. A header is supplied at the top of the columns to further clarify the quantities in the table. For the pure rotational bands ($\Delta\nu = 0$), $\gamma_{air}$ values from the HITRAN2008 listing were retained. For the 2-0 band and
beyond, high accurate (±3%) N₂-broadening measurements for the P(3) and P(6) lines of
2-0 band by Chou et al. [10] were used to calibrate the Meredith and Smith measurements
for the 2-0 band [11]. The calibrated results were then scaled to air by $\gamma_{air} = 0.9\gamma_{N₂}$. The same $\gamma_{air}$ was applied to the corresponding bands of DF.

$\gamma_{self}$: The self-broadening parameters in the HITRAN2008 listing, which were based on Pine
and Fried [12], were retained for the fundamental and $\Delta \nu = 1$ bands. For the first overtone
and $\Delta \nu = 2$ bands, the high accurate (±2%) diode laser measurements by Chou et al. [13]
for P(3) and P(6) lines were used to calibrate the previous Meredith measurements [14].
Linear extrapolation against the vibrational level $\nu$ were made using the measurements of
Pine and Fried [12] and Chou et al. [13] to obtain $\gamma_{self}$ for the other bands. The same $\gamma_{self}$
was applied to the corresponding bands of DF.

$n$: For the pure rotational, fundamental and $\Delta \nu = 0, 1$ bands, $n$ values from the HITRAN2008
listing were retained. A default value of 0.5 was used for bands with $\Delta \nu \geq 2$.

Shift: Values from the HITRAN2008 listing were retained for the pure rotational, fundamental
and $\Delta \nu = 0, 1$ bands. Measurements by Guelachvili and Smith [15] were used for the
bands with $\Delta \nu \geq 2$.

**HCl/DCl**

$\gamma_{air}$: For the fundamental band, the air-broadening parameters for HCl in the HITRAN2008
compilation turned out to be fitted not with a Voigt profile, but with the Galatry profile
based on the Pine and Looney [9] measurements. However, the Dicke narrowing
parameter was not provided in the previous database. In the same manner as for HF as
mentioned above, the corresponding collisional, or Dicke, narrowing parameters have been
cast into a separate columnar table that is easily linked to the main part of HITRAN using
the unique combination of: molecule number, isotopologue number, and quantum
identifications. A header is supplied at the top of the columns to further clarify the
quantities in the table.

The N₂ and O₂ broadening parameters of the R(3) transition of the 0-0 band has been
measured accurately by Park et al. [16]. Applying $\gamma_{air} = 0.79\gamma_{N₂} + 0.21\gamma_{O₂}$, Pine and
Looney measurements were multiplied by a factor of 0.960 to obtain the air broadening
parameters for 0-0 band. In a similar fashion, high accurate measurements (±1% for N₂-
and O₂- broadening) for the P(4) and R(3) lines of 2-0 band by De Rosa et al. [17] were
used to scale Pine and Looney measurements with a factor of 1.089. The scaled values
were used for bands with $\Delta \nu \geq 2$. 
$\gamma_{self}$: For the pure rotational, fundamental and $\Delta v = 0,1$ bands, Pine and Fried [12] measurements were combined with Hurtmans et al. [18] accurate measurement for the P(14) line to extrapolate to high-$J$ lines. For the $\Delta v = 2$ bands, Pine and Fried measurements were scaled with high accurate measurements (±3% accuracy) of Ortwein et al. [19] and De Rosa et al. [17]. Ogilvie and Lee [20] and Zughul et al. [21] measurements were used for the $\Delta v = 3$ and $\Delta v \geq 4$ bands, respectively. Tudorie et al. [22] refitting of the $\gamma_{self}$ measurements by Eaton and Thompson [23] were used for all bands of DCl.

$n$: Pine and Looney [9] $n$ values were used for $\Delta v \geq 1$ bands. For the pure rotational band, the $n$ values measured by Park et al. [16] for R(3), 0.71; by Drouin [24] for R(0), 0.73 agree very well with the Pine and Looney $n$ values of 0.71 and 0.74 for R(3) and R(0), respectively. Thus, Pine and Looney values were also used for the pure rotational bands.

Shift: It was found that the air shift for the same rotational line of different vibrational bands has a linear dependence on the transition frequencies as shown in Fig. 3. Adopting the slope derived from this figure, we extrapolated Pine and Looney measurements of $\delta_{air}$ for the 1-0 band to other bands.

Figure 3: Air-induced shift for H$^{35}$Cl.
**HBr/DBr**

$\gamma_{air}$: Values from the HITRAN2008 listing were retained for HBr. The same values were applied to DBr.

$\gamma_{self}$: Values from the HITRAN2008 listing was retained for HBr. Benedict and Herman [25] calculated values were used for all band of DBr.

$n$: No data were available. A default value of 0.5 was used.

*Shift*: No data were available.

**HI/DI**

$\gamma_{air}$: For the fundamental, first, second, third overtone and corresponding $\Delta v = 1, 2, 3, 4$ bands, $\gamma_{N_2}$ from Domanskaya et al. [26] was scaled to air by $\gamma_{air} = 0.9 \gamma_{N_2}$. For the pure rotational band, the values from the fundamental band were used. For $\Delta v \geq 5$ bands, the values from the 4-0 band were used. $\gamma_{air}$ for HI were used for DI.

$\gamma_{self}$: Hartmann et al. accurate measurements [27] for $\gamma_{self}$ were used for 1-0, 2-0 and $\Delta v = 1, 2$ bands. Bulanin et al. [28] recent $\gamma_{self}$ measurements were used for $\Delta v \geq 3$ bands. $\gamma_{self}$ for HI were used for DI.

$n$: No data were available. A default value of 0.5 was used.

*Shift*: Domanskaya et al. [26] accurate measurements for the N$_2$ shift were adopted for HI. No data were found for the DI air shift.

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**References:**


[4] Guelachvili G, Niay P, Bernage P. Fourier transform high-resolution measurements on the $2 \leftarrow 0$, $3 \leftarrow 0$, $4 \leftarrow 0$, $5 \leftarrow 0$ infrared absorption bands of HI and DI. J Mol Spectrosc 1981;85:253-70.


[29] PGOPHER, a Program for Simulating Rotational Structure, C. M. Western, University of Bristol, http://pgopher.chm.bris.ac.uk