Rotational quenching of H$_2$CO by molecular hydrogen: cross-sections, rates, pressure broadening.

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ABSTRACT

We compute the rotational quenching rates of the first 81 rotational levels of ortho- and para-H$_2$CO in collision with ortho- and para-H$_2$, for a temperature range of 10-300 K. We make use of the quantum close-coupling and coupled-states scattering methods combined with the high accuracy potential energy surface of Troscompt et al. (2009a). Rates are significantly different from the scaled rates of H$_2$CO in collision with He; consequently, critical densities are noticeably lower. We compare a full close-coupling computation of pressure broadening cross sections with experimental data and show that our results are compatible with the low temperature measurements of Mengel & De Lucia (2000), for a spin temperature of H$_2$ around 50 K.

Key words: Astrochemistry, molecular processes, molecular data, ISM: molecules

1 INTRODUCTION

In order to relate quantitatively the observed rotational spectra and the molecular abundances, knowledge of the relative importance of photon induced transitions and collision induced transitions is imperative. While the Einstein $A$ and $B$ coefficients can be obtained experimentally (see e.g. the JPL and CDMS databases Drouin (2012); Müller et al. (2005)), the rates of molecular collisional excitation/quenching need to be calculated with help of precise microscopic frameworks. Many molecular quenching rates have been put forward in the last 40 years, either for molecular collisions with He or for collisions with H, electrons and H$_2$. In many types of interstellar regions, especially so when molecular complexity is present, the main collider is molecular hydrogen, H$_2$. Recently, a renewed large effort has been devoted to compute the rotational quenching rates of molecules by H$_2$ (see references in the review by Van der Tak (2011)) and most collisional data are available in the BASECOL Dubernet et. al. (2012) and LAMDA Schöier et al. (2005) databases. Special emphasis was put on molecules specific to the Herschel Space Observatory, and among them, water. However, complex organic molecules continue to play a prominent role in the understanding of proto-stellar evolution as well as being probes for various interstellar environments.

Among all organic molecules, formaldehyde (H$_2$CO) is especially abundant, since it is the first stable molecule resulting from the hydrogenation of the ubiquitous CO molecule (Peters et al. 2011). Being abundant and displaying a large range of both transition frequencies and energy levels, formaldehyde is a tool of choice to probe the physical conditions of the gaseous interstellar matter (Maret et al. 2004 Kama et al. 2013). By using models that do not suppose Local Thermodynamical Equilibrium (LTE), it is possible to reach reliable estimates of the molecular abundance of H$_2$CO together with the other parameters of the gas, its temperature and density (Ceccarelli et al. 2003 Van der Tak et al. 2007). The famous formaldehyde “anomalous” absorption was also shown to provide a probe of the ortho-to-para ratio of H$_2$ (Troscompt et al. 2009b) and a distance-independent tracer of the cosmic star formation history (Darling & Zeiger 2012).

Several computations of the excitation rates of H$_2$CO have been proposed in the literature. Excitation by He atoms, being easier to perform, has been used for long as a model for excitation by H$_2$, even if it is known for being an underestimation of unknown precision (Green et al. 1978 Green 1991 Sharma et al. 2012). In our group, we computed (Troscompt et al. 2009a) the quenching rates of H$_2$CO by H$_2$, but only for the low levels of excitation of ortho-formaldehyde (only the first 10 levels) and for low kinetic temperatures ($T \lesssim 100$ K). These computations were based on a high precision Potential Energy Surface (PES) for the van der Waals interaction H$_2$CO – H$_2$. In the present paper, we extend our previous computations to a much broader range of rotational energies and temperatures, for both ortho- and para-H$_2$CO, using the same PES. Also, in order to assess the precision of this PES, we compare experimental pressure broadening cross sections measured by

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O and CO (Drouin & Wiesenfeld 2012b; Faure et al. 2011). The rotational basis set is devised as follows. For all scattering energies, if $J_{K_aK_c}$ is the last open channels, the $J' = J + 1, J + 2$ values were added to the basis. However, since a given $J$ rotational number spans a large amount of rotational energy, rotational levels were capped, at $E_{\text{max}} = 400 \text{ cm}^{-1}$ for collision energies $E_{\text{coll}} \lesssim 175 \text{ cm}^{-1}$, and increasing progressively to $E_{\text{max}} = 1200 \text{ cm}^{-1}$ for $E_{\text{coll}} \sim 1000 \text{ cm}^{-1}$. These large values of $E_{\text{max}}$ are needed to converge cross sections; a similar effect was previously observed for methyl-formate colliding with Helium (Faure et al. 2011).

The rotational basis for ortho-H$_2$ is $J_2 = 1$. It has been shown for many systems that including $J_2 = 3$ in the basis does not have a noticeable influence for temperatures as low as 300 K (e.g. Daniel, Dubernet & Grosjean (2011)). The rotational basis for para-H$_2$ proved difficult to settle. We were able to use the $J_2 = 0, 2$ basis set for CC para-H$_2$ - ortho-H$_2$CO collisions, with $E_{\text{coll}} \lesssim 130 \text{ cm}^{-1}$ (Troscompt et al. 2009a). For para-H$_2$CO, because of the level structure, the $J_2 = 0, 2$ basis for CC computations proved to be practically impossible for $E_{\text{coll}} \gtrsim 50 \text{ cm}^{-1}$. As a result, we resorted only to a $J_2 = 0$ basis, both for ortho- and para-H$_2$CO, stretching the CC computations as high as possible and continuing with the CS approximation. In order to assess the importance of the $J_2 = 2$ channel, however, we complemented the ortho-H$_2$CO data with a full CS $J_2 = 0, 2$ computation up to $E_{\text{coll}} \sim 900 \text{ cm}^{-1}$, using a coarse energy grid. This allowed us to check $i)$ that cross sections for transitions with $J_2 = 2 \rightarrow 0$ are negligible, $ii)$ that cross sections for transitions with $J_2 = 2 \rightarrow 2$ are very similar to those with $J_2 = 1 \rightarrow 1$ (as observed for other systems, see e.g. Daniel, Dubernet & Grosjean (2011)) and $iii)$ that the difference between the basis sets $J_2 = 0$ and $J_2 = 0, 2$ decreases with increasing collision energy, from an average of $\sim 30\%$ to below 10\%.

Because of the large number of expansion terms of the potential function in the spherical harmonic basis (Troscompt et al. 2009a), several strategies have been devised in order to converge the inelastic scattering computations in a reasonable amount of time (We arbitrarily tried to limit ourselves to 72 hours of clock time, for one energy scattering point, on 12 CPU cores). The radial propagation used a step size parameter steps = 15 except at collision energies below 10 cm$^{-1}$ where was steps progressively increased up to 50. Also, rmax values were progressively increased in the

1 This is the MOLSCAT convention, differing from usual spectroscopic conventions by the ordering of the axes.

2 Repository at [http://ipag.osug.fr/~afaure/molscat/index.html](http://ipag.osug.fr/~afaure/molscat/index.html)
low-energy regime from default to 100. Other propagation parameters were taken as the MOLSCAT default values.

For total energies above approximately 330 cm\(^{-1}\) the coupled channels (CC) approach, exact in the fully converged limit, proved to be impractical. We thus had to resort to the usual coupled states (CS) approximation, with all its shortcomings. Like in our recent HDO-H\(_2\) rate calculations (Wiesenfeld, Scribano & Faure 2011), we used an additive constant to scale appropriately the CS cross sections by their factors of difference. The statistics of difference \(\delta\) between the CC and CS cross sections was also examined. We found the following values (in \(\text{Å}^2\), \(s\), the standard deviation): \(<|\delta|\) \(\leq 0.5\), \(s(\delta) \leq 2\). Also, for collisions with ortho-H\(_2\), the total angular momentum \(J_{\text{tot}}\) was not stepped by unit values, as is done usually. For CC calculation above \(E_{\text{coll}} > 200\) cm\(^{-1}\), a step in \(J_{\text{tot}}\) value \(J_{\text{STEP}} = 4\) was used, with a careful checking of the convergence of the \(J_{\text{STEP}} > 1\) procedure. This procedure was used throughout the CS computations.

The energy grid was chosen to guarantee a good description of the resonances, including those pertaining to the high lying rotational states. Also, since we aim at rates for temperatures up to 300 K, a particular care was taken to ensure both some economy in the computational load and a good convergence of the rate computation. Let us recall that the quenching rate from state \(i\) to state \(j\), \(k_{j\rightarrow i}(T)\) (in cm\(^3\) sec\(^{-1}\)) is related to the inelastic cross section \(\sigma_{j\rightarrow i}(E)\) (in \(\text{Å}^2\), with \(E\), the collision energy) by the well known Boltzmann average:

\[
k_{j\rightarrow i}(T) = \sqrt{8 \frac{1}{\pi \mu T^3}} \int_0^\infty \sigma_{j\rightarrow i}(E) E \exp(-E/T) dE, \quad (1)
\]

where \(T\) and \(E\) are expressed in the same units, and \(\mu\) is the collisional reduced mass. The probability density \(E \exp(-E/T)\) going very slowly down with energy, it is customary, for calculating \(k_{j\rightarrow i}(T = T_0)\), to compute \(\sigma_{j\rightarrow i}(E)\) up to \(E \sim 10 T_0\) (e.g., Dubernet et al. 2009). This approach is prohibitively time-intensive for a heavy molecule like H\(_2\)CO, even within the CS approximation. For high lying rotational states, we inspected carefully the actual numerical convergence of equation (1) and stopped our energy grid as soon as the rate was saturated by 10% in general, and 25% for the highest levels, with \(E_{\text{top}} > 150\) cm\(^{-1}\).

The computation of the pressure broadening cross-sections (Wiesenfeld & Faure 2010; Drouin & Wiesenfeld 2012b) necessitates a very fine energy grid and a good control of the elastic cross sections, much more difficult to obtain than the corresponding inelastic sections. Hence, we had to re-calculate all the \(S\)-matrices with collision energies from 2 to 70 cm\(^{-1}\). Then, we compute the \(\sigma_{\text{PB}}(T)\) in order to compare with the experimental results of Mengel & De Lucia (2000), in a temperature range of 10 – 30 K. Both collisions with para-H\(_2\) (basis set, \(J_2 = 0, 2\)) and ortho-H\(_2\) (basis set, \(J_2 = 1\)) were performed on an identical fine energy grid and in the CC formalism.

### 3 RESULTS AND DISCUSSION

#### 3.1 Cross sections

The inelastic cross sections have a general shape that is similar to all earlier findings, for collisions of a molecule with H\(_2\). As usual, the inelastic scattering with \(J_2 = 0\) may be markedly different from the scattering with \(J_2 > 0\). This was observed and thoroughly discussed for H\(_2\)O and HDO scattering computations (Dubernet et al. 2009; Daniel, Dubernet & Grosjean 2011; Wiesenfeld, Scribano & Faure 2011; Faure et al. 2012), and observed for a wide range of other collisions, SO\(_2\) and Cl atoms being recent examples (Cernicharo et al. 2011; Lique & Alexander 2012). Experiments with H\(_2\) colliding with water molecules also extensively confirm this difference (Drouin & Wiesenfeld 2012b; Yang et al. 2011).

The situation with formaldehyde colliding with H\(_2\), \(J_2 = 0\) and \(J_2 > 0\) is however less clear, as some ortho-H\(_2\) and para-H\(_2\) collisions are nearly identical, especially for small sections and large \(\Delta J\). In particular, the pressure broadening of H\(_2\)CO is very important, for calculating \(k_{j\rightarrow i}(T)\) going very slowly down with energy, it is customary, for calculating \(k_{j\rightarrow i}(T = T_0)\), to compute \(\sigma_{j\rightarrow i}(E)\) up to \(E \sim 10 T_0\) (e.g., Dubernet et al. 2009). This approach is prohibitively time-intensive for a heavy molecule like H\(_2\)CO, even within the CS approximation. For high lying rotational states, we inspected carefully the actual numerical convergence of equation (1) and stopped our energy grid as soon as the rate was saturated by 10% in general, and 25% for the highest levels, with \(E_{\text{top}} > 150\) cm\(^{-1}\).

#### 3.2 Rates

All quenching rates for all levels of table 1 are computed for the same temperature grid as Green (1991), 10 K \(\leq T \leq 300\) K. The full table is deposited in the LAMDA database (Schöier et al. 2005) and BASECOL database (Dubernet et al. 2012), and may be asked to the authors. The rates with ortho-H\(_2\) are based on the \(J_2 = 1\) sections only. In all cases, rates with para-H\(_2\) are given as a Boltzmann average over the populations of \(J_2 = 0, 2\), with the further approximation of \(\sigma(E_{\text{coll}}; J_2 = 2) \approx \sigma(E_{\text{coll}}; J_2 = 1)\), when necessary (see above). The influence of the \(J_2 = 2\) initial states may indeed be very large, as was also observed, in another context, for the pressure broadening of H\(_2\)O by H\(_2\) (Drouin & Wiesenfeld 2012b).

Figure 4 compares globally present critical densities and critical densities from Green (1991), for electric-dipole allowed transitions. We compare our present rates with para-H\(_2\) with the properly scaled rates with He. We have the following definition on the critical density \(n^*\):

\[
n^*_i = \sum_{j < i} A_{j\rightarrow i} k_{j\rightarrow i}(T) \quad (2)
\]

where \(i\) is the level under scrutiny and \(j^*\) denotes all levels connected by a radiative transition, while \(j\) spans all levels. Left panel shows the scatter of critical densities ratios at \(T = 300\) K, while on the right panel, all ratios are averaged and plotted against temperature. The scatter is moderate, with no ratio exceeding 3. The right panels shows the evolution of
3.3 Pressure broadening

In order to assess the reliability of the PES, we found it useful to compare measured and computed pressure-broadening cross sections, $\sigma^{\text{Br}}(T)$ (Wiesenfeld & Faure 2010; Drouin & Wiesenfeld 2012b; Faure et al. 2013). The main advantage of pressure broadening is that experiments and computations held both absolute quantities, with no scaling involved, rendering the comparison very meaningful. Unfortunately, only a very limited set of $\text{H}_2\text{CO}$ pressure broadening data exists for an $\text{H}_2$ buffer gas (Mengel & De Lucia 2000), for very low temperatures. The experimental results for the $2_{12} \rightarrow 3_{13}$ transition are depicted in figure 3 along with full CC calculations of $\sigma^{\text{Br}}(T)$. We see that the para-$\text{H}_2$ and ortho-$\text{H}_2$ computation bracket the experimental values, which are very well simulated by an ortho-to para-$\text{H}_2$ ratio (OPR) corresponding to a pseudo-equilibrium at $\sim 50\ K$, corresponding to a OPR of 0.27. That the OPR of $\text{H}_2$ may vary during the collisional cooling experiment has been proved with cell walls covered with anamorphic water (Drouin & Wiesenfeld 2012b). Nothing is known for formaldehyde, and discussion with the authors of Mengel & De Lucia (2000) could not settle the case. We remain thus with a good plausibility argument, as long as the pressure broadening experiments with $\text{H}_2$ are not fully characterized.

### Table 1. $\text{H}_2\text{CO}$ rotational levels, in cm$^{-1}$. The experimental values are from Bocquet et al. (1996); the MOLSCAT values are calculated via the rotational constants described in the text.

| Level | $J$ | $K_A$ | $K_C$ | MOLSCAT | Experimental | Level | $J$ | $K_A$ | $K_C$ | MOLSCAT | Experimental |
|-------|----|------|------|---------|-------------|-------|----|------|------|---------|-------------|
| 1     | 0  | 0    | 0    | 0.00000 | 0.00000    | 1     | 1  | 1    | 1    | 10.53897 | 10.53900    |
| 2     | 1  | 0    | 1    | 2.42961 | 2.42960    | 2     | 1  | 1    | 0    | 10.70021 | 10.70010    |
| 3     | 2  | 0    | 2    | 7.28640 | 7.28640    | 3     | 2  | 1    | 2    | 15.23672 | 15.23690    |
| 4     | 3  | 0    | 3    | 14.56547 | 14.56550   | 4     | 2  | 1    | 1    | 15.72044 | 15.72020    |
| 5     | 4  | 0    | 4    | 24.25953 | 24.25970   | 5     | 3  | 1    | 3    | 22.28172 | 22.28220    |
| 6     | 5  | 0    | 5    | 36.35981 | 36.35920   | 6     | 3  | 1    | 2    | 23.24914 | 23.24870    |
| 7     | 6  | 0    | 6    | 47.32780 | 47.32760   | 7     | 4  | 1    | 4    | 31.67285 | 31.67290    |
| 8     | 6  | 0    | 6    | 47.32780 | 47.32760   | 8     | 4  | 1    | 3    | 33.28429 | 33.28350    |

the average ($n_i^*$) as a function of $T$. For higher temperatures, the effect of $\text{H}_2$ being different of He diminishes, since higher collisions energies are more sensitive to the hard walls of the target, where the potential grows exponentially (repulsion of the wave functions). $\text{H}_2$ and He become more similar, and the rates tend one towards the other.
4 DISCUSSION - CONCLUSION

It is important to know which errors are to be expected, and to have some clues on how these errors might influence astrophysical modeling. We expect the error on the rates $k(T)$ to be uniformly increasing from low lying levels to higher lying ones, and also from low to medium temperatures. Quantifying this error is very risky, as errors may arise from all the phases of the rate computation: \textit{ab initio} computation, fits and long distance behavior of the PES, convergence of the CC/CS procedures, convergence of the averaging procedure of the sections with collision energy.

Internal consistency with our earlier approach (Troscompt et al. 2009a) show differences less than 10\%, for $J < 5$, $T < 50$ K. This shows that the convergence error in this domain cannot exceed 20-30\%. In the high temperature domain ($T \geq 150$ K), it is safe to assume errors much larger than 30\%, because of the poor convergence of formula \textit{(1)}, but still within a factor 2. The magnitude of the $\delta$ values as well as the similarities between the $J_2 = 1 \rightarrow 1$ and $J_2 = 2 \rightarrow 2$ plead in favor of such a conservative value, as does the convergence of critical densities between our work and the previous collisions with He by Green (1991).

Accuracy of the PES is very difficult to assess, without any firm experimental comparison, like has been done for H$_2$O and to a lesser extent CO (Yang et al. 2011). Drouin \& Wiesenfeld (2012b) Faure et al. 2013. Chefdeville et al. (2012). Our results are, however, compatible with measurements of Mengel \& De Lucia (2000). Because of the great importance and ubiquity of the formaldehyde molecule, further experiments would give indications on the precision of the PES and convergence procedures used in this paper.

The relevance of the ortho-to-para ratio of H$_2$ has been stressed several times already, as it may be of crucial importance in order to correctly model the astrophysical environments. While the difference in rates for ortho-H$_2$ and para-H$_2$ is large for low lying levels at low energies, see Troscompt et al. (2009b) for an application, this difference decreases at larger transition energies, as the hard walls of the PES play a more important role than the long range behavior. Indeed, the main increase in $\sigma(J_2 > 0)$ with respect to $\sigma(J_2 = 0)$ is due to the averaging out of the quadrupolar moment and dipolar polarizability of H$_2$ in its ground rotational states. The same is true, up to a global scale, for the difference in behavior between He and ortho-H$_2$.

Extension of these computations to higher levels and higher temperatures is by no means a difficult task, on the physics point of view, because of the rigid rotor structure of H$_2$CO, its first bending frequency (the out-of-plane bend) arising at 1167.3 cm$^{-1}$ (Clouthier \& Ramsay 1983). The true limiting factor arises from numerical load, with very large $N \times N$ matrices to invert and propagate ($N > 2000$). The same situation arises for the excitation of heavier complex organic molecules, like methyl formate or dimethyl ether, which display many spectral lines very far from LTE, in various spectral surveys like Caux et al. (2011). Unfortunately, quasi classical trajectories methods are limited for all those cases because of ambiguities arising in the subsequent quantization of rotational levels (Faure \& Wiesenfeld 2004). Use of very large grid of computers and combinations of OpenMP/mpi approaches may overcome these difficulties.

We have calculated an extensive set of low to medium temperature quenching rates, for all levels of H$_2$CO below 210 cm$^{-1}$. These rates are ready to be incorporated in the various non-LTE models for the interstellar medium. At low temperatures, differences with earlier rates of H$_2$CO colliding with Helium are very important and they remain noticeable at all temperatures, with ratios up to 50\% at 300 K, where they are the most similar. Since Troscompt et al. (2009a) was tailored to be very precise at low temperatures for ortho-H$_2$CO, we still recommend to use those rates for applications at $T \leq 30$ K. The present rates should have a large importance on the inferring of H$_2$CO column densities, away from LTE conditions.

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Figure 1. (Color online) Cross-sections (upper three panels) and rates (lower three panels) for three widely observed quenching transitions of ortho-H$_2$CO (first column: $2_{11} \rightarrow 1_{10}$, at $E_{up} = 22.62$ K; second column: $4_{32} \rightarrow 3_{31}$, at $E_{up} = 140.93$ K; third column: $7_{35} \rightarrow 6_{34}$, at $E_{up} = 203.9$ K). In all panels the red (dashed) line denotes the H$_2$ rotational $J_2 = 0$ initial and final state, the blue (solid) line, the same with $J_2 = 1$ and the black (dashed-dotted), the same with $J_2 = 2$. The red dash-dotted rates include the influence of the population of the $J_2 = 2$ para state of H$_2$ (see text). Rates and sections with $J_2 = 0 \leftrightarrow J_2 = 2$ are two or three orders of magnitude lower and not depicted. Rates for collisions with Helium [Green 1991] are the lowest rates in all three inferior panels (green color online). Note that for cross sections, for sake of clarity, the energy is the total energy. Note also that cross sections display usual resonance patterns which are not conspicuous at this log scale.
Figure 2. Left panel: ratio of critical densities (eq. [2], present work to Green [1991]) properly scaled, for all levels, at $T = 300$ K. Right panel, average over all critical densities ratios, as a function of temperature. Both panels: open squares, ortho-H$_2$CO with para-H$_2$ ($J_2 = 0$) or He; filled diamonds para-H$_2$CO with para-H$_2$ ($J_2 = 0$) or He.
Figure 3. (Color online) Pressure broadening of the $2_{12} \rightarrow 3_{13}$ transition. Red symbols, measurements of [Mengel & De Lucia (2000)]. Dashed and dot-dashed lines, present computations with respectively ortho-H$_2$ and para-H$_2$. Full line, ortho-to-para of H$_2$ equivalent to a spin temperature of 50 K.