HAL open science

Collisional excitation and dissociation of HCl by H

François Lique, Alexandre Faure

To cite this version:

François Lique, Alexandre Faure. Collisional excitation and dissociation of HCl by H. Monthly Notices of the Royal Astronomical Society, 2017, 472 (1), pp.738–743. 10.1093/mnras/stx2025 . hal-01917993

HAL Id: hal-01917993

https://hal.science/hal-01917993v1

Submitted on 1 Oct 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Distributed under a Creative Commons Attribution 4.0 International License

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS **472,** 738–743 (2017)
Advance Access publication 2017 August 5

doi:10.1093/mnras/stx2025

Collisional excitation and dissociation of HCl by H

François Lique[1★] and Alexandre Faure[2]

[1]*LOMC – UMR 6294, CNRS-Université du Havre, 25 rue Philippe Lebon, BP 1123 – F-76 063 Le Havre cedex, France*
[2]*Université Grenoble Alpes, CNRS, IPAG, F-38000 Grenoble, France*

Accepted 2017 August 3. Received 2017 August 3; in original form 2017 July 11

ABSTRACT

Among interstellar chlorine bearing molecules, HCl is certainly the most useful probe for studying chlorine chemistry since it is formed at the end of the reaction network. Accurate knowledge of the HCl abundance in the interstellar medium requires the calculation of excitation rate coefficients of HCl due to collisions with the most abundant collisional partners. Following the recent calculations of HCl–He, HCl–H_2 and HCl–electron rotational rate coefficients, we report here theoretical calculations of the HCl–H collisional data. Fully quantum time-independent rate coefficients for the collisional excitation of HCl by H are provided for temperature ranging from 10 to 500 K. The strongest collision-induced rotational HCl transitions are those with $\Delta j = 1$ and the magnitude of the HCl–H rate coefficients is larger than that of the HCl–H_2 ones. In addition, we also provide rate coefficients for the collisional dissociation of HCl by H, another astrophysically relevant process. Below 300 K, it is found that the destruction of HCl induced by collisions with H is much faster than previously considered in astrochemical models. As a first application, we simulate the excitation of HCl by H_2 and H in typical protostellar shock conditions. We show that hydrogen atoms significantly increase the simulated line intensities, suggesting HCl abundance lower than currently estimated.

Key words: molecular data – molecular processes – ISM: abundances.

1 INTRODUCTION

In the interstellar medium (ISM), three chlorine bearing molecules,[1] HCl (Blake, Keene & Phillips 1985), H_2Cl^+ (Luca et al. 2012) and HCl^+ (Lis et al. 2010; Neufeld et al. 2012), have been detected. These hydrides are expected to contain a significant fraction of chlorine in space. In high-density regions of the ISM where hydrogen is predominantly molecular, HCl is even expected to be the main gas phase chlorine reservoir (Neufeld & Wolfire 2009). In more diffuse regions, chlorine is mostly atomic (in the form of Cl^+) and the abundance of the three chlorine hydrides are expected to be quite similar (Neufeld & Wolfire 2009), containing a few per cent of the elemental chlorine cosmic abundance (n(Cl)/n(H) $\sim 3 \times 10^{-7}$).

Among these chlorine bearing molecules, HCl is certainly the most useful tool for studying chlorine chemistry since it is formed at the end of the reaction path for the synthesis of chlorine bearing species. In addition, Schilke, Phillips & Wang (1995) have shown that HCl can be used as a tracer of very dense regions ($>10^7$ cm^{-3}), thanks to its relatively large dipole moment and high critical density. Hence, HCl can be considered as a key molecule for studying the physical and chemical conditions of the ISM.

In the dense ISM, HCl was first identified by Blake et al. (1985). Recently, thanks to the heterodyne instrument for the far-infrared (HIFI) on board the Herschel Space Observatory, HCl emission spectra have been detected from a significant number of star forming regions (Codella et al. 2012; Kaźmierczak-Barthel et al. 2014; Kama et al. 2015). In particular, HCl emission was observed towards the protostellar shock L1157-B1 (Codella et al. 2012) and these observations provided new insight into the chlorine chemistry in dense and warm ($T > 150$ K) regions. The HCl abundance was thus found to be $\simeq$3–6 $\times 10^{-9}$ relative to H_2, suggesting that HCl is actually a negligible reservoir of chlorine in star-forming regions and that chlorine is locked up in other species. Such a low HCl abundance is also in good agreement with that derived from observations towards low- and high-mass protostars by Peng et al. (2010).

In the diffuse ISM, HCl was recently detected towards W31C (Monje et al. 2013). The $j = 1 \rightarrow 0$ lines of the two stable HCl isotopologues, $H^{35}Cl$ and $H^{37}Cl$, were observed in absorption. The analysis of Monje et al. (2013) suggests that HCl accounts for $\simeq$0.6 per cent of the total gas-phase chlorine, which exceeds the predictions by a large factor based on astrochemical models, thus confirming previous results by Lis et al. (2010).

While the analysis of absorption lines from diffuse clouds is straightforward (the excitation temperatures are close to the cosmic

★ E-mail: francois.lique@univ-lehavre.fr

[1] Some metal halides with chlorine, NaCl, AlCl and KCl, have also been detected in the circumstellar gas towards the late-type carbon star IRC+10216 (Cernicharo & Guelin 1987).

© 2017 The Authors
Published by Oxford University Press on behalf of the Royal Astronomical Society

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021

microwave background radiation ∼2.73 K), accurate estimation of HCl abundance from emission lines requires the use of collisional rate coefficients with the most abundant interstellar species, namely e^-, He, H and H_2. Rate coefficients for the rotational/hyperfine excitation of HCl by He atoms (employed as a substitute for H_2) have been calculated by Neufeld & Green (1994) several years ago and revisited recently by Lanza & Lique (2012).[2] In the absence of collisional data with H and H_2, the dominant collisional partners in the ISM, HCl–H and HCl–H_2 rate coefficients were generally extrapolated from HCl–He data. However, it is well known that such approach can be quite inaccurate, in particular for molecular hydrides (Roueff & Lique 2013), and it seems crucial to determine the actual HCl–H and HCl–H_2 rate coefficients.

Then, we have computed accurate rate coefficients for rotational/hyperfine excitation of HCl by collisions with H_2 molecules for temperatures ranging from 5 to 300 K (Lanza & Lique 2014; Lanza et al. 2014a,b). The rate coefficients were derived from extensive quantum calculations using a new accurate potential energy surface (PES) obtained from highly correlated *ab initio* approaches. As expected, significant differences were found between HCl–H_2 and HCl–He rate coefficients. In particular, Lanza et al. (2014b) showed that the use of the H_2 rate coefficients significantly increase the simulated HCl line intensities. As a consequence, the HCl abundance derived from the observations is significantly reduced by the use of the actual H_2 rate coefficients. These new rate coefficients were used in the analysis of surveys of HCl confirming the low HCl abundance in protostellar cores $\sim 10^{-10}$ (Kama et al. 2015). Assuming that chlorine depletes by at least two orders of magnitude into (yet unknown) refractory reservoirs of chlorine on grains, astrochemical models can reproduce such a low gas-phase HCl abundance (Kama et al. 2015).

To gain more insight into the HCl abundance in protostellar regions where both H and H_2 are abundant, it is also crucial to determine HCl–H collisional data. Such calculations are challenging since two processes are in competition during collisions between HCl and H: the inelastic and reactive (both hydrogen exchange and destruction of HCl) processes. This is explained by the reactive nature of the H_2Cl system. The obtention of accurate collisional data requires to consider simultaneously both processes during the calculations.

Recently, we overcame this difficult problem and presented quantum mechanical calculations of cross-sections for the rotational excitation of HCl by H, including the Cl + H_2 reactive channels (Lique 2015, hereafter Paper I) using the state-of-the-art PES of Bian & Werner (2000). Thus, in addition to inelastic cross-sections, accurate data for the destruction of HCl induced by collisions with H were also provided. Such data are also useful to model the abundance of chlorine in chemical kinetic models. In this paper, we use the collisional cross-sections for the collisional excitation and dissociation of HCl by H from Paper I to compute the temperature variation of the rate coefficients for rotational excitation and dissociation of HCl by H. Then, we briefly discuss the impact of these new data on both the chlorine chemistry and the HCl abundance determination in the ISM.

This paper is organized as follows: Section 2 briefly describes the calculations. The results are presented and discussed in Section 3. In Section 4, we discuss the astrophysical consequences of the new collisional and reactive rate coefficients. Conclusions are drawn in Section 5.

[2] Yang & Stancil (2014) also computed HCl–He rate coefficients for a large range of temperatures but neglected the hyperfine structure.

2 THEORETICAL APPROACH

In this paper, j designates the rotational level of HCl. During a collision between HCl and H, three processes compete:

1) The inelastic process:

$$\mathrm{HCl}(j) + \mathrm{H}' \rightarrow \mathrm{HCl}(j') + \mathrm{H}' \quad (1)$$

2) The exchange process:

$$\mathrm{HCl}(j) + \mathrm{H}' \rightarrow \mathrm{H}'\mathrm{Cl}(j') + \mathrm{H} \quad (2)$$

3) The reactive process:

$$\mathrm{HCl}(j) + \mathrm{H}' \rightarrow \mathrm{Cl} + \mathrm{HH}' \quad (3)$$

In the last process, we explicitly consider the H_2 rotational structure but the results were summed over the final rotational states of H_2. In our study, HCl molecules were restricted to their ground vibrational state $v = 0$. Inelastic and reactive cross-sections for the above three processes have been published in Paper I. We refer the reader to Paper I for full details on the scattering calculation. In summary, calculations were performed with the ABC program (Skouteris et al. 2001) using the fully quantum time-independent close coupling approach. The ClH_2 PES of Bian & Werner (2000) calculated at the internally contracted multireference configuration interaction level using large atomic basis set was used. Calculations were carried out for collision energies up to at least 2500 cm^{-1}. Collisions between H and HCl in its first 11 ($j = 0 - 10$) rotational states were considered. In the calculations, all rotational and vibrational levels of the diatomic (either H_2 or HCl) moiety were included subject to the exclusion of (a) levels with internal energy greater than ∼14 000 cm^{-1} and (b) levels in which the angular momentum quantum number j of the diatomic moiety is greater than 21. The energy levels were determined theoretically from the ClH_2 PES of Bian & Werner (2000). The hyperfine structure of the HCl molecules due to coupling between the rotational quantum number j and the nuclear spin of the Cl atom was not considered explicitly in the scattering calculations in order to save computing time. Hyperfine resolved rate coefficients were obtained from rotationally resolved data using infinite order sudden (IOS) approaches (see below). In addition, the calculations were performed using the atomic mass of ^{35}Cl. However, the results can be safely used for analysis of $H^{37}Cl$ spectra since we do expect a very minor impact of the isotopic substitution on the magnitude of the rate coefficients.

From the astrophysical point of view, rotational excitation through inelastic or exchange process cannot be distinguished so that, in the following, the inelastic and exchange cross-sections were summed. Hence, we refer hereafter to only two processes, namely, the collisional excitation of HCl (inelastic + exchange processes) and the collisional dissociation of HCl (reactive process).

From the calculated cross-sections, one can obtain the corresponding thermal rate coefficients at temperature T by an average over the collision energy (E_c):

$$k_{\alpha\rightarrow\beta}(T) = \left(\frac{8}{\pi\mu k_B^3 T^3}\right)^{\frac{1}{2}} \times \int_0^\infty \sigma_{\alpha\rightarrow\beta}\, E_c\, \mathrm{e}^{-\frac{E_c}{k_B T}}\, \mathrm{d}E_c \quad (4)$$

where $\sigma_{\alpha\rightarrow\beta}$ is the cross-section from initial state α (HCl(j) + H) to final state β (HCl(j') + H or Cl + H_2), μ is the reduced mass of

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021

the system and k_B is the Boltzmann's constant. Calculations up to 2500 cm^{-1} allow determining rate coefficients from 10 to 500 K.

3 RESULTS

3.1 Collisional excitation of HCl by H

First, we focus on the collisional excitation process. Fig. 1 displays the temperature variation of the rate coefficients for the rotational de-excitation of HCl($j = 1 - 4$) by H to HCl($j = 0$) (upper panel) and of HCl($j = 2 - 5$) by H to HCl($j = 1$) (lower panel). The complete set of (de)excitation rate coefficients is available online from the LAMDA (Schöier et al. 2005) and BASECOL (Dubernet et al. 2013) websites.

As expected, the rate coefficients decrease with increasing Δj. The strongest collision-induced rotational HCl transitions are the transitions with $\Delta j = 1$. More generally, we observe a propensity rules in favour of transitions with odd Δj because of the strong anisotropy of the HCl–H PES with respect to the H approach. We also note the relatively large magnitude of the rate coefficients ($k(T) > 10^{-10}$). Such a magnitude can certainly be explained by the large well depth seen in the HCl–H PES (∼155 cm^{-1}) which efficiently allowed for collisional excitation of HCl induced by H. Hence, one can anticipate that HCl will be efficiently excited through collisions with H in the ISM.

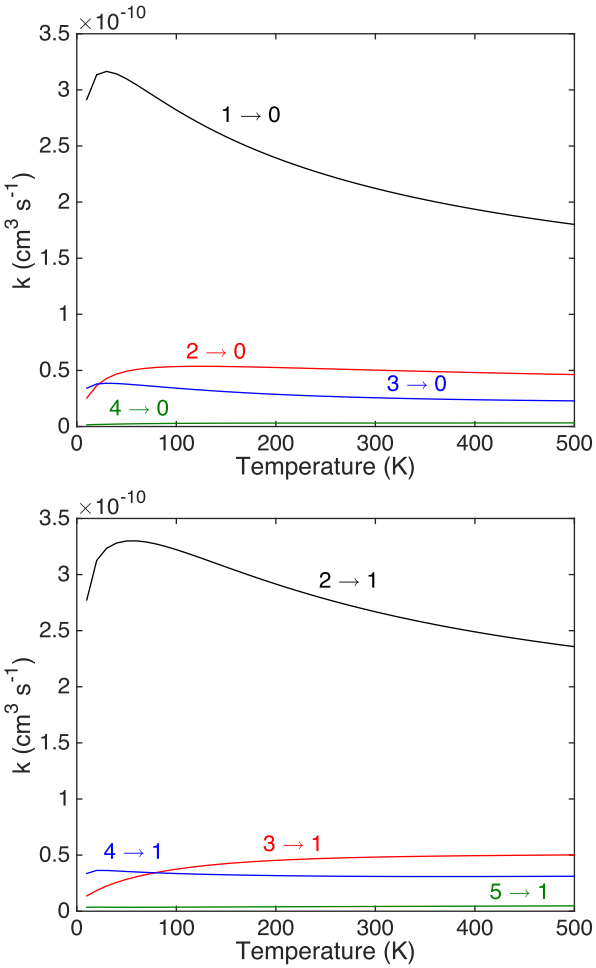

Figure 1. Typical variation with temperature of the rotational de-excitation rate coefficients of HCl by H.

Then, it is interesting to compare the present rate coefficients with those reported recently for the rotational excitation of HCl by He (Lanza & Lique 2012) and H_2 (Lanza et al. 2014b). The three sets of rate coefficients were computed at a similar level of accuracy so that, in this comparison, we expect to probe the impact of the different collisional partners. In astrophysical applications, when collisional data are not available, it is quite usual to estimate the rate coefficients of a colliding system from the values calculated for the same molecule in collision with another colliding partner (usually the He collisional partner). The methodology which is generally used (Lique et al. 2008) consist in assuming that the excitation cross-sections are similar for both systems. The rate coefficients are then derived by correcting only for the change in reduced mass which appears in equation (4), which lead to the following scaling relationship:

$$k^{\mathrm{H}} \simeq 1.9 \times k^{\mathrm{He}} \simeq 1.4 \times k^{\mathrm{H_2}} \tag{5}$$

It is now well established that rate coefficients for collisions with para- and ortho-H_2 are generally very different (Roueff & Lique 2013) and the above scaling relationship is expected to apply better to collisions with para-H_2.

In Fig. 2, we compare the HCl–H, HCl–He and HCl–H_2 (both para- and ortho-H_2) rate coefficients for a selected number of transitions.

He and H_2 rate coefficients have been already compared in details in Lanza et al. (2014b) and differences up to an order of magnitude have been found, especially at low temperatures. We focus here on the comparisons implying the new collisional data with the H collisional partner. First of all, one can see that the rate coefficients for collisions with H have the highest magnitude as expected from the scaling relationships. However, especially at low temperature, the new data are up to an order of magnitude larger than the He or para-H_2 data, exceeding by a large factor what is predicted from the simple scaling relationship. We also note that the differences depend on the transitions and on the temperature leading to the impossibility of extrapolating H collisional data from He or H_2 collisional data. Hence, it confirms that, for hydrides, it is unrealistic to estimate unknown collisional rate coefficients by simply applying a scaling factor to the existing rate coefficients. This result was previously observed for water (Daniel et al. 2015) and ammonia (Bouhafs et al. 2017).

Finally, in HCl, the coupling between the nuclear spin ($I = 3/2$) of the chlorine atom[3] and the molecular rotation results in a weak splitting (Alexander & Dagdigian 1985) of each rotational level j into four hyperfine levels (except for the $j = 0$ level which splits into only one level and for the $j = 1$ level which splits into only three levels). Each hyperfine level is designated by a quantum number F ($F = I + j$) varying between $|I - j|$ and $I + j$.

In most of the low-j astronomical spectra, the hyperfine structure of the HCl molecules is resolved (Kama et al. 2015). Hyperfine resolved HCl–H rate coefficients can be deduced from the rotationally resolved rate coefficients as described in Faure & Lique (2012):

$$k_{jF\to j'F'}(T) = \frac{k^{\mathrm{IOS}}_{jF\to j'F'}(T)}{k^{\mathrm{IOS}}_{j\to j'}(T)} k_{j\to j'}(T), \tag{6}$$

[3] Both ^{35}Cl and ^{37}Cl display the same nuclear spin.

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021

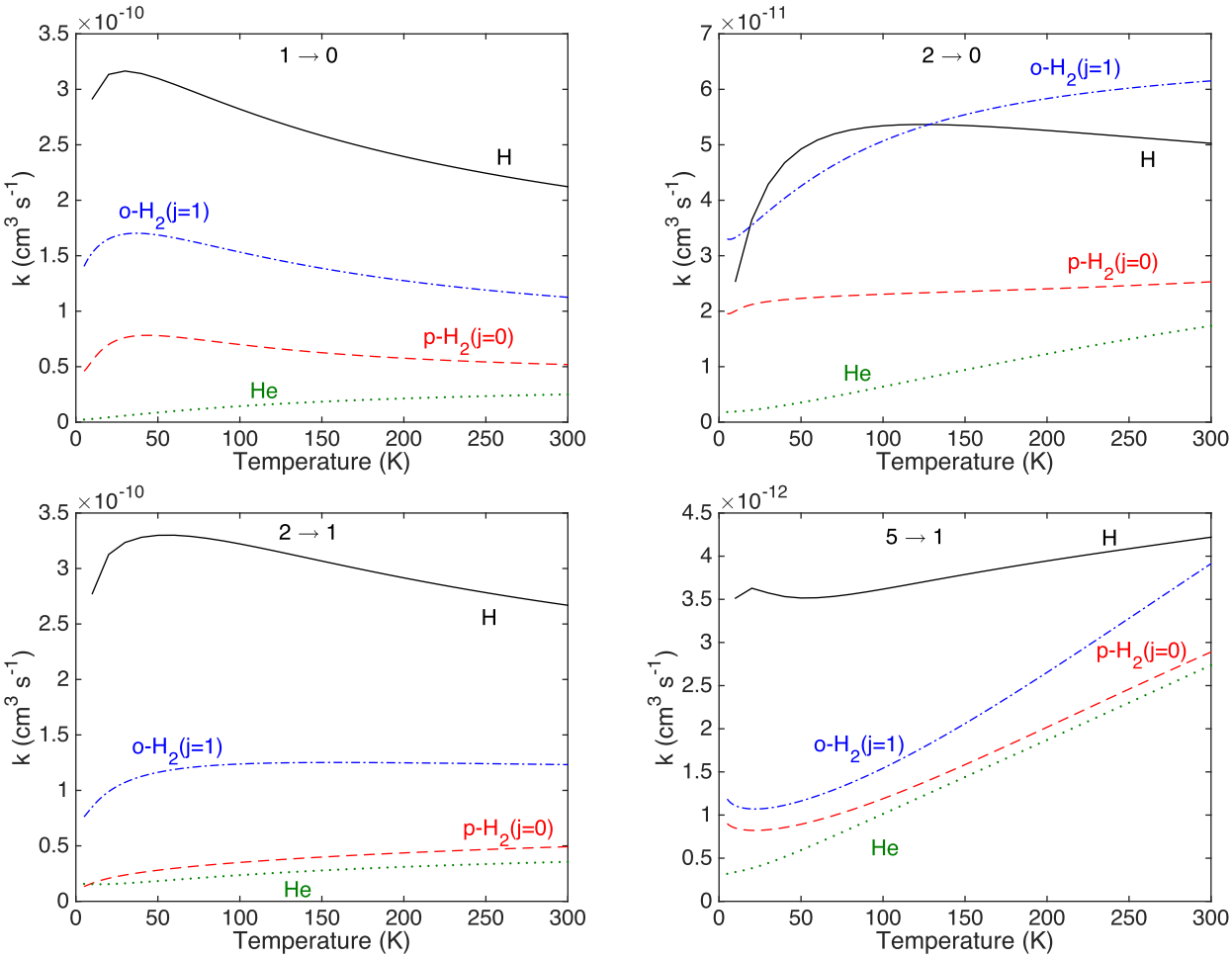

Figure 2. Comparison between HCl–H, HCl–He and HCl–H_2 (both para- and ortho-H_2) rate coefficients.

$k^{\rm IOS}_{j\to j'}(T)$ and $k^{\rm IOS}_{jF\to j'F'}(T)$ (IOS stands for infinite order sudden) can be calculated as follows (e.g Corey & McCourt 1983):

$$k^{\rm IOS}_{j\to j'}(T) = (2j'+1)\sum_L \begin{pmatrix} j' & j & L \\ 0 & 0 & 0 \end{pmatrix}^2 (2L+1)k_{L\to 0}(T) \qquad (7)$$

and

$$k^{\rm IOS}_{jF\to j'F'}(T) = (2j+1)(2j'+1)(2F'+1) \times \sum_L \begin{pmatrix} j' & j & L \\ 0 & 0 & 0 \end{pmatrix}^2 \times \begin{Bmatrix} j & j' & L \\ F' & F & I \end{Bmatrix}^2 k_{L\to 0}(T), \qquad (8)$$

where ( ) and { } are, respectively, the '3-j' and '6-j' Wigner symbols. In equations (7) and (8), the rotationally resolved rate coefficients computed above are used for the $k_{L\to 0}(T)$ rate coefficients.

The complete set of hyperfine resolved rate coefficients is also available online from the LAMDA (Schöier et al. 2005) and BASECOL (Dubernet et al. 2013) websites.

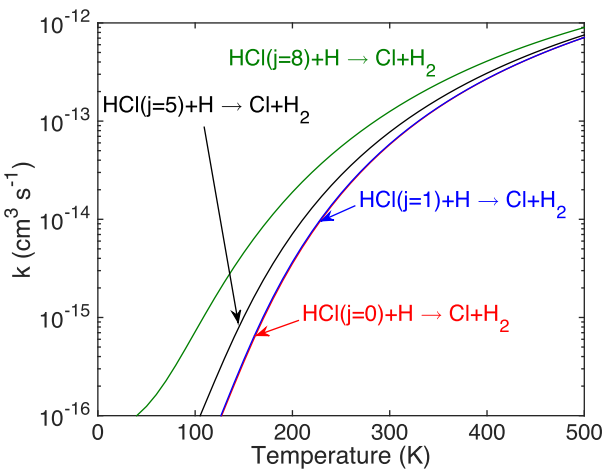

Figure 3. Temperature variation of the rate coefficients for the collisional dissociation of HCl(j) by H.

3.2 Collisional dissociation of HCl by H

We also present the results for the collisional dissociation of HCl by H. Fig. 3 presents the temperature variation of the rate coefficients for the collisional dissociation of HCl(j) by H.

It can be easily seen that the reactive rate coefficients for the destruction of HCl by H increase rapidly with increasing temperature,

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021

as expected for an abstraction reaction with a significant energy barrier (∼2500 K). At temperatures above ≃300 K, the rate coefficients are larger than 10^{-13} cm^3 s^{-1}, consequently the reaction is relatively efficient (especially considering the high abundance of H in astrophysical media).

We do observe an increase of the rate coefficients with increasing rotational state of the reactant at low temperatures. Indeed, the internal energy of the reactive system increases with increasing rotational levels and this leads to an enhancement of the reaction rate coefficients through tunnelling effect. At higher temperatures, the collisional dissociation of HCl(j) by H rate coefficients tends to be similar whatever the initial rotational state of HCl is.

4 ASTROPHYSICAL APPLICATIONS

4.1 The excitation of HCl in protostellar shocks

As a first application and in order to test the impact of the new collisional excitation rate coefficients, we have performed radiative transfer calculations to simulate the excitation of HCl in protostellar shock conditions. HCl was detected by Codella et al. (2012) *via* the $j = 1 \rightarrow 0$ transition at 626 GHz towards the L1157-B1 shock. This source coincides with the near-infrared H_2 'knot A' where the fraction of atomic hydrogen is high, $n(\mathrm{H})/n(\mathrm{H_2}) \sim 0.3$, as shown by Nisini et al. (2010). This suggests that the shock is partially dissociative. L1157-B1 therefore provides an excellent template to study the impact of our H collisional data. We do not intend, however, to quantitatively model the *Herschel* observations of Codella et al. (2012), which is clearly beyond the scope of our work.

Non-local thermodynamic equilibrium (non-LTE) radiative transfer calculations were performed with the RADEX code (van der Tak et al. 2007) using the escape probability formalism approximation for an expanding sphere. We focus here on the brightness temperature of the $j = 1 \rightarrow 0$ transition using either (i) only the H_2 collisional partner or (ii) both the H and H_2 collisional partners. The only radiation field is the cosmic microwave background (CMB) at 2.73 K.

The physical conditions are taken from Codella et al. (2012): we consider an HCl column density of 10^{13} cm^{-2}, a kinetic temperature of 200 K, a density of H_2 fixed at 3×10^5 cm^{-3} and a density of H of 1×10^5 cm^{-3} corresponding to a fraction H/H_2 ∼ 0.3. Finally, H_2 was assumed to lie in the ground para- and ortho-rotational states $j_{\mathrm{H_2}} = 0$ and $j_{\mathrm{H_2}} = 1$, respectively, with the following ortho-to-para ratios (OPR): (i) OPR = 0 (H_2 lies in $j_{\mathrm{H_2}} = 0$ only) and (ii) OPR = 3 (statistical limit). We note that the OPR of H_2 was actually measured along the L1157-mm outflow where it was found to vary between ∼ 0.6 and 2.8, i.e. it is always below the equilibrium value of 3. Fig. 4 shows the results of our radiative transfer calculations.

As one can see the brightness temperature obtained when including the H collisional partner is significantly higher than that obtained with H_2 only. The ratio between the corresponding line intensities is ≃1.5–2. Such an increase is due to the large HCl–H rate coefficients that significantly contribute to the excitation of HCl, as illustrated in Fig. 2. The HCl–H rate coefficients are indeed up to an order of magnitude larger than those of H_2. This is why hydrogen atoms, even if not the dominant colliding partner, significantly increase the population of the excited level and this extra population translates into a higher brightness temperature as we are in the optically thin regime.

The present calculations thus show that the HCl abundance derived from radiative transfer analysis performed using only the H_2 collisional partner can be overestimated by up to a factor of ∼2, depending on the H/H_2 fraction. It is then crucial to revise the HCl abundance in protostellar shocks using the new collisional data.

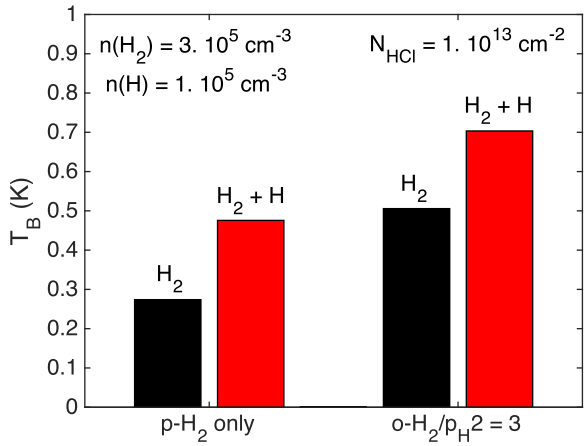

Figure 4. HCl brightness temperature for the $j = 1 \rightarrow j' = 0$ line with and without the H collisional partner.

4.2 Thermal rate coefficient for the dissociation of HCl by H

In astrochemical kinetic models, the rotational structure of the reactants and of the products are usually neglected. Consequently, what is needed is a 'thermal' rate coefficient $k(T)$ summed over the product states and averaged over the reactant states, assuming a Maxwell–Boltzmann thermal distribution for the latter:

$$k(T) = \frac{\sum_j (2j+1)\mathrm{e}^{-\epsilon_j/kT} k_j(T)}{Q}$$
$$Q = \sum_j (2j+1)\mathrm{e}^{-\epsilon_j/kT}, \quad (9)$$

where ϵ_j is the energy of the jth rotational level. We have employed our state-to-state rate coefficients to compute the thermal rate coefficient for the dissociation of HCl by H. In practice the sums in equation (9) run over to the range $j = 0$–10 covered by our quantum calculations, which guarantees that the thermal rate coefficient is converged up to $T_k = 500$ K.

In Fig. 5, we present the temperature variation of the thermal rate coefficient computed in this work for the collisional dissociation of HCl by H. Fig. 5 also presents the rate coefficient currently used in astrochemical models. It was adopted by Neufeld & Wolfire (2009) following the recommendation of Kumaran, Lim & Michael (1994) who performed a fit to various experimental measurements for the reverse reaction Cl + H_2 → HCl + H in the temperature range T_k = 199–2939 K (Kumaran et al. 1994).

As one can see significant difference exist between the 'reference' rate coefficient and our result. At low temperatures, the destruction of HCl by H is much faster (by orders of magnitude) than expected from the (extrapolated) fit of Kumaran et al. (1994). The flattening of the rate coefficient below 100 K can be attributed to the tunnelling effect that significantly enhances the reactivity at collision energies below the barrier. Unfortunately, there is to our knowledge no experimental data available in this temperature regime. The large increase of the rate coefficient means that the HCl + H reaction could play a role even at low temperature if the fraction of hydrogen atoms is high enough. At temperatures higher than 200 K, the agreement between our results and the recommendation of Kumaran et al. (1994) is quite satisfactory. The small discrepancies (a factor of ∼2) could

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021

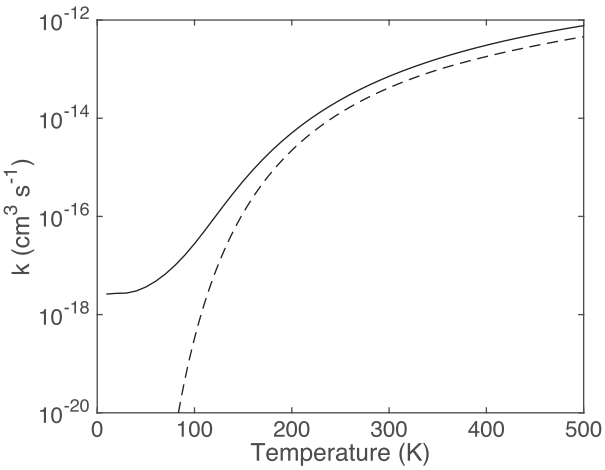

Figure 5. Comparison between present (solid line) and the reference (dashed line) thermal rate coefficient for the destruction of HCl through the HCl+H reaction. See the text for details.

Table 1. Thermal rate coefficients for the collisional dissociation of HCl by H.

Temperature (K)	k (cm^3 s^{-1})
10	2.62×10^{-18}
20	2.71×10^{-18}
30	2.74×10^{-18}
50	3.65×10^{-18}
70	6.69×10^{-18}
100	2.78×10^{-17}
150	5.24×10^{-16}
200	5.03×10^{-15}

reflect some uncertainties in the experimental equilibrium constant for $Cl+H_2 \rightleftharpoons HCl + H$ (Kumaran et al. 1994).

The theoretical rate coefficient was fitted to the Arrhenius–Kooij formula in the 200–500 K temperature range which we recommend for use in astrochemical models:

$$k(T) = 8.76 \times 10^{-12} \left(\frac{T}{300}\right)^{0.89} \exp\left(-\frac{1443}{T}\right) \quad (10)$$

Below 200K, this fit is not accurate because of the strong tunnelling effect and we therefore provide the data in the range 10–200 K in Table 1.

5 CONCLUSION

We have presented quantum mechanical calculations of rate coefficients for the collisional excitation and dissociation of HCl by H. The results show that HCl can be easily excited through collisions with H. We also found that, at low temperature, HCl is destroyed through collisions with H much more rapidly than what is presently considered in astrochemical models.

In order to evaluate the effect of the new excitation data on the astrophysical modelling, we have performed radiative transfer calculations for the typical physical conditions of protostellar shocks where HCl has been detected. The simulated brightness temperatures obtained considering both the H and H_2 collisional partners are significantly larger than the ones obtained considering only the H_2 collisional partner. This result suggests a further decrease of the HCl column density in partially dissociative shocks so that the abundance of HCl may be even lower than recently reported by Codella et al. (2012). This reinforces the conclusion of these authors that HCl is a minor chlorine carrier in star-forming regions.

ACKNOWLEDGEMENTS

This research was supported by the Agence Nationale de la Recherche (ANR-HYDRIDES), contract ANR-12-BS05-0011-01. Support by the Programme National 'Physique et Chimie du Milieu Interstellaire' (PCMI) of CNRS/INSU with INC/INP co-funded by CEA and CNES is also acknowledged. FL acknowledges financial support from the Institut Universitaire de France.

REFERENCES

Alexander M. H., Dagdigian P. J., 1985, J. Chem. Phys., 83, 2191
Bian W., Werner H.-J., 2000, J. Chem. Phys., 112, 220
Blake G. A., Keene J., Phillips T. G., 1985, ApJ, 295, 501
Bouhafs N., Rist C., Daniel F., Dumouchel F., Lique F., Wiesenfeld L., Faure A., 2017, MNRAS, 470, 2204
Cernicharo J., Guelin M., 1987, A&A, 183, L10
Codella C. et al., 2012, ApJ, 744, 164
Corey G. C., McCourt F. R., 1983, J. Phys. Chem., 87, 2723
Daniel F., Faure A., Dagdigian P. J., Dubernet M.-L., Lique F., Forêts G. P. d., 2015, MNRAS, 446, 2312
Dubernet M.-L. et al., 2013, A&A, 553, A50
Faure A., Lique F., 2012, MNRAS, 425, 740
Kama M. et al., 2015, A&A, 574, A107
Kaźmierczak-Barthel M., van der Tak F. F. S., Helmich F. P., Chavarría L., Wang K.-S., Ceccarelli C., 2014, A&A, 567, A53
Kumaran S. S., Lim K. P., Michael J. V., 1994, J. Chem. Phys., 101, 9487
Lanza M., Lique F., 2012, MNRAS, 424, 1261
Lanza M., Lique F., 2014, J. Chem. Phys., 141, 164321
Lanza M., Kalugina Y., Wiesenfeld L., Lique F., 2014a, J. Chem. Phys., 140, 064316
Lanza M., Kalugina Y., Wiesenfeld L., Faure A., Lique F., 2014b, MNRAS, 443, 3351
Lique F., 2015, J. Chem. Phys., 142, 241102 (Paper I)
Lique F., Tobola R., Kłos J., Feautrier N., Spielfiedel A., Vincent L. F. M., Chałasiński G., Alexander M. H., 2008, A&A, 478, 567
Lis D. C. et al., 2010, A&A, 521, L9
Luca M. D. et al., 2012, ApJ, 751, L37
Monje R. R., Lis D. C., Roueff E., Gerin M., De Luca M., Neufeld D. A., Godard B., Phillips T. G., 2013, ApJ, 767, 81
Neufeld D. A., Green S., 1994, ApJ, 432, 158
Neufeld D. A., Wolfire M. G., 2009, ApJ, 706, 1594
Neufeld D. A. et al., 2012, ApJ, 748, 37
Nisini B., Giannini T., Neufeld D. A., Yuan Y., Antoniucci S., Bergin E. A., Melnick G. J., 2010, ApJ, 724, 69
Peng R., Yoshida H., Chamberlin R. A., Phillips T. G., Lis D. C., Gerin M., 2010, ApJ, 723, 218
Roueff E., Lique F., 2013, Chem. Rev., 113, 8906
Schilke P., Phillips T. G., Wang N., 1995, ApJ, 441, 334
Schöier F. L., van der Tak F. F. S., van Dishoeck E. F., Black J. H., 2005, A&A, 432, 369
Skouteris D. et al., 2001, J. Chem. Phys., 114, 10662
van der Tak F. F. S., Black J. H., Schöier F. L., Jansen D. J., van Dishoeck E. F., 2007, A&A, 468, 627
Yang B., Stancil P. C., 2014, ApJ, 783, 92

This paper has been typeset from a TEX/LATEX file prepared by the author.

Downloaded from https://academic.oup.com/mnras/article/472/1/738/4067806 by guest on 01 October 2021