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# Collisional excitation of HD by H

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## ABSTRACT

The HD molecule plays an important role in many astrophysical environments. Accurate modelling of the gas cooling induced by HD and its abundance in such media requires a proper modelling of its excitation by both radiative and collisional processes. Reliable state-to-state collisional rate coefficients in extended temperature regimes are then essential to allow for the description of different astrophysical environments where deviations from local thermodynamic equilibrium regime can occur. Here, we report exact quantum time-independent reactive scattering calculations for the ro-vibrational excitation of HD by H. Rate coefficients are computed for temperatures up to 5000 K and transitions between all ro-vibrational states with internal energies up to  $14,000\text{ cm}^{-1}$ . Previous results neglecting reactive and exchange channels of the colliding system are compared to the new ones and significant differences are found. The present work represents a big step in the complete description of the HD–H collisional system, in terms of rovibrational states considered, temperature range explored and accuracy. Hence, we recommend the use of the new HD–H collisional data presented here to accurately model the astrophysical environments where HD plays a role.

**Key words:** Molecular data – Molecular processes – Scattering – Early Universe

## 1 INTRODUCTION

The HD molecule is prevalent in many astrophysical environments. HD observations directly trace the density of molecular hydrogen which represents a key parameter to better understand the star formation processes and galaxy evolution (Kennicutt & Evans 2012). Measuring the HD column density also enables the determination of the D/H elemental abundance ratio (Neufeld et al. 2006).

Possible deviation from its primordial nucleosynthesis value, observationally confirmed by Levshakov et al. (2002), is crucial for constraining the chemical evolution of interstellar molecular clouds. Indeed, at high redshifts, HD is used to constrain the cosmic-ray ionization rate (Balashev & Kosenko 2020; Kosenko et al. 2021), cosmic rays being the main source of HD formation in the interstellar medium (ISM).

In protoplanetary disks, HD has a high abundance relative to H<sub>2</sub>. Molecular hydrogen being the most dominant species in such media, HD is thus found to be a promising tracer of the disks mass (McClure et al. 2016; Trapman et al. 2017). The modelling of HD emission spectra in protoplanetary disks would also bring valuable information about the planets formation process.

Moreover, it is now well established that both H<sub>2</sub> and its isotopic form HD play a crucial role in the evolution of the early

Universe chemistry (Puy et al. 1993; Galli & Palla 1998; Stancil et al. 1998; Galli & Palla 2002; Lepp et al. 2002; Glover & Abel 2008; Coppola et al. 2011; Longo et al. 2011; Coppola et al. 2012). Specifically, HD is the primary coolant of the primordial gas at temperatures lower than 100 K, metals being not yet present at high redshifts.

For the same reason, molecular hydrogen in its pure and isotopic variants are key coolants of the compressed gas in pregalactic shocks and low metallicity clouds (Shapiro & Kang 1987; Machida et al. 2005; Johnson & Bromm 2006; Shchekinov & Vasiliev 2006; Nakauchi et al. 2014; Coppola et al. 2016). Hence, they play an important role in the determination of the mass, composition and lifetimes of the first stellar objects formed in our Universe (Schleicher et al. 2013; Hirano et al. 2015; Sugimura et al. 2016).

A complete knowledge about the excitation conditions of the HD molecule is crucial to accurately derive HD abundance in ISM from observational spectra and to describe the cooling mechanisms of pristine gas. In such astrophysical environments, physical conditions are extreme and deviations from local thermodynamic equilibrium (LTE) are prevalent (Roueff & Lique 2013a). Hence, models describing the chemical, thermal and gravitational evolution of the gas strongly relies on accurate collisional rate coefficients.

Helium and hydrogen, both in atomic and molecular forms, are the most dominant collisional partners in the interstellar medium. In the early Universe, atomic hydrogen is the dominant species. Notably because of their high astrophysical interest, numerous ex-

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perimental and theoretical studies of HD in collision with helium and molecular hydrogen have been carried out over the past fifty years (Itikawa & Takayanagi 1972; Itikawa 1974; Chu 1975; Gentry & Giese 1977; Roueff & Zeppen 1999; Flower & Roueff 1999a; Nolte et al. 2012; Sultanov et al. 2012, 2016; Croft et al. 2018; Wan et al. 2019).

Excitation of HD through collisions with atomic hydrogen received less attention. Indeed, the reactive nature of this collisional system lead to more complex theoretical modelling. Current astrophysical models generally relies on the rate coefficients provided by Flower & Roueff (1999a). In their inelastic scattering study, Flower & Roueff (1999a) neglected the reactive and hydrogen exchange channels that are inhibited by a barrier height of approximately  $3500 \text{ cm}^{-1}$  (Mielke et al. 2002a). In the light of recent studies (Lique & Faure 2012; Lique 2015a), neglecting the reactive channels is highly questionable as significant inaccuracies in the rate coefficients can arise from such treatment. Recently, Desrousseaux et al. (2018) carried out reactive scattering calculation for the rotational excitation of HD by H. In this work, they considered the first 11 rotational levels of HD and provided rate coefficients for temperatures up to 1000 K. They showed that while the most dominant rate coefficients ( $\Delta j = 1$ ) were in good agreement with the results by Flower & Roueff (1999b), up to an order of magnitude of differences can be found for the other transitions at temperatures higher than 300 K. More recently, Zhou et al. (2021) computed highly accurate rate coefficients for the inelastic, reactive, and hydrogen exchange processes in rovibrationally excited collisions of HD( $v = 1, j = 0 - 5$ ) with H (where  $v$  and  $j$  respectively denote the vibrational and rotational states of the HD molecule). They provided rate coefficients for temperatures up to 1000 K and noted also significant differences with previous results by Flower & Roueff (1999b) for transitions involving  $\Delta j > 2$ .

HD is an important constituent of primordial gas and is observed in a wide variety of astrophysical environments, from the coldest (e.g. ISM) to the warmest (e.g. protoplanetary disks) where rovibrationally excited states of HD are populated. Being able to accurately describe the state-to-state excitation of HD with the most abundant species in a wide variety of physical conditions is hence crucial. The present work extends previous reactive scattering calculations by Desrousseaux et al. (2018) and Zhou et al. (2021), both in terms of rovibrational states considered and in the temperature range explored. In this paper, we present quantum-mechanical reactive scattering calculations of collisional rate coefficients of the HD–H system, covering temperatures up to 5000 K and rovibrational levels of the HD molecule up to  $14,000 \text{ cm}^{-1}$  (HD( $v = 3, j = 10$ )).

The paper is organised as follows: Section 2 describes the computational details of the scattering study. Results are presented in Section 3. Summary and concluding remarks are drawn in Section 4.

## 2 METHODS

In our investigation of the scattering dynamics, we used the  $\text{H}_3$  potential energy surfaces (PES) by Mielke et al. (2002b). The ab initio PES was computed at the full configuration interaction (FCI) level of theory using a complete basis set extrapolation and has been shown to provide theoretical  $\text{H}_2$ –H thermal rate coefficients (Lique et al. 2014; Mielke et al. 2003) that perfectly match with the experimental data. We used the ABC reactive scattering code from Skouteris et al. (2000) to carry out close coupling calculations of the cross sections for the inelastic (Eq. 1), exchange (Eq. 2) and

reactive (Eq. 3) processes:



that are all possible during the collisions even if processes 2 and 3 are inhibited by a large activation barrier of  $3500 \text{ cm}^{-1}$ .

As discussed by Tao & Alexander (2007), it is computationally efficient to choose basis functions which are eigenfunctions of the operator corresponding to the interchange of the two hydrogen atoms. Since the Hamiltonian is symmetric with respect to interchange of the two hydrogens, there will be no coupling between odd (*ortho*) and even (*para*) rotational states of  $\text{H}_2$ , so that the number of reactive channels that lead to the formation of the  $\text{H}_2$  molecule is reduced by a factor of  $\sim 2$ . Following the methodology detailed by Tao & Alexander (2007), we then obtained inelastic, exchange and reactive cross sections. Cross sections were computed for all ro-vibrational levels with internal energies lower than  $14,000 \text{ cm}^{-1}$ . To ensure convergence of the cross sections, we considered in the close-coupling calculations all channels corresponding to levels of the molecule (HD or  $\text{H}_2$ ) with internal energy lower than  $26,000 \text{ cm}^{-1}$ , excluding those for which the rotational angular momentum  $j$  is greater than 22. Calculations were done for all values of the total angular momentum  $J$  that made a non-zero contribution to inelastic, exchange and reactive processes and the projection quantum number of the total angular momentum  $k$  was restricted to 9.

From the inelastic, exchange or reactive cross sections  $\sigma_{vj \rightarrow v'j'}(E_c)$ , the corresponding rate coefficients at temperature  $T$  were obtained by averaging over the collision energy ( $E_c$ ):

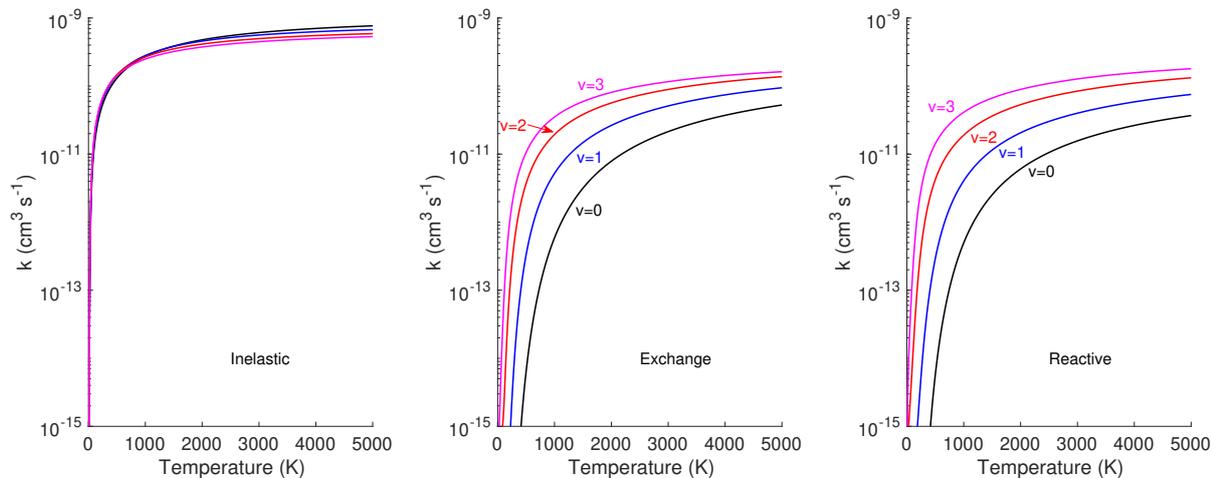
$$k_{vj \rightarrow v'j'} = \left( \frac{8}{\pi \mu k_B^3 T^3} \right)^{\frac{1}{2}} \times \int_0^\infty \sigma_{vj \rightarrow v'j'} E_c e^{-\frac{E_c}{k_B T}} dE_c, \quad (4)$$

where  $v$  and  $j$  respectively correspond to the vibrational and rotational states of HD in the entrance channel and  $v'$  and  $j'$  correspond to the vibrational and rotational state of the molecule in the exit channel (HD or  $\text{H}_2$ ).  $\mu$  is the reduced mass of the colliding system and  $k_B$  is the Boltzmann's constant. Calculation of the cross sections up to total energies (internal plus kinetic energies) of  $\sim 41,500 \text{ cm}^{-1}$  allow us to determine rate coefficients up to 5000 K. The complete set of de-excitation rate coefficients are given as a supplementary data to this article.

## 3 RESULTS

In Figure 1, we present the temperature variation of the rate coefficients for the inelastic, reactive and exchange processes in HD( $v, j = 0$ )–H collisions, summed over all possible final rovibrational states. As already observed (Desrousseaux et al. 2018), for the pure rotational excitation of HD( $v = 0, j = 0$ ) the inelastic process is significantly dominant over all the explored temperature range, the reactive and exchange processes being negligible at low temperature and at least two orders of magnitude lower at high temperature. Such behaviour can be attributed to the large activation barrier ( $\sim 3500 \text{ cm}^{-1}$ ) needed to be overcome for these two reactive processes.

Rate coefficients for inelastic collisions summed over all possible final rovibrational states do not significantly depend on the



**Figure 1.** Temperature variation of the rate coefficients for the inelastic, exchange, and reactive processes (summed over all final states) for collisions of  $\text{HD}(v, j = 0)$  with H.

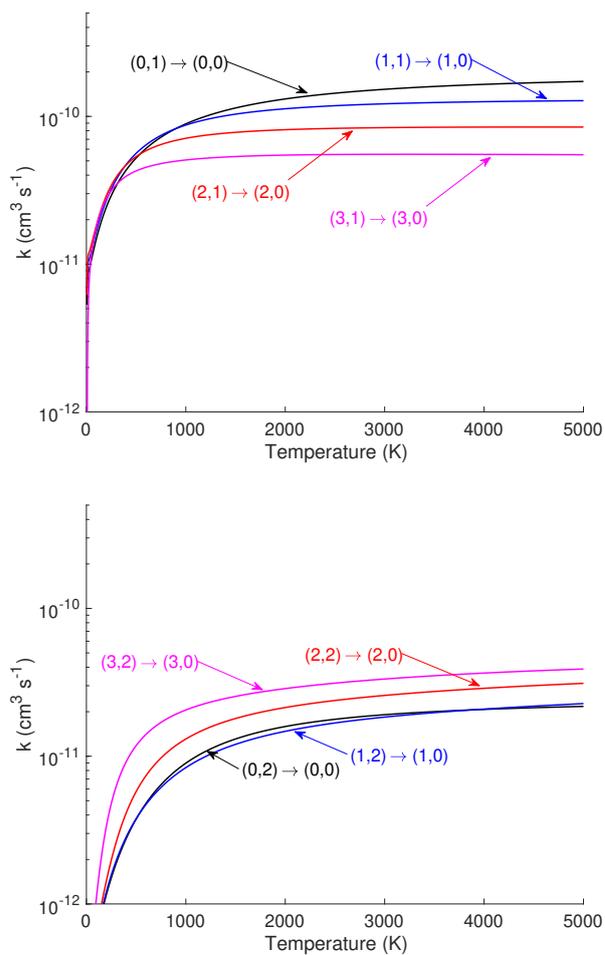
initial vibrational state of the HD molecule: their magnitude only slightly decreases with increasing initial vibrational state at high temperature and conversely at low temperature. However, the exchange and reactive rate coefficients, which are almost identical in magnitude, significantly increase with increasing initial vibrational state of HD. The same behaviour is observed for the  $\text{H}_2\text{-H}$  reactive collisions and it can be explained by the lowering of the activation barrier with the vibrational excitation of the reagent molecule (Lique 2015b; Barg et al. 1981). Vibrationally excited HD exchange and reactive processes start to compete with the inelastic process for temperatures higher than 1000 K, with differences being as low as less than a factor 4 between inelastic and exchange/reactive rate coefficients for  $\text{HD}(v = 3, j = 0)$  at 3000 K. Such findings clearly show that reactive and exchange channels can perturb the pure inelastic process and thus should be included when describing the collisions between HD and H.

In this paper, we focus on the collisional excitation of HD by H. Collisional excitation through inelastic or exchange processes can not be distinguished from an astrophysical point of view. Hence, in the following, the inelastic and exchange cross sections have been summed before computing the excitation rate coefficients.

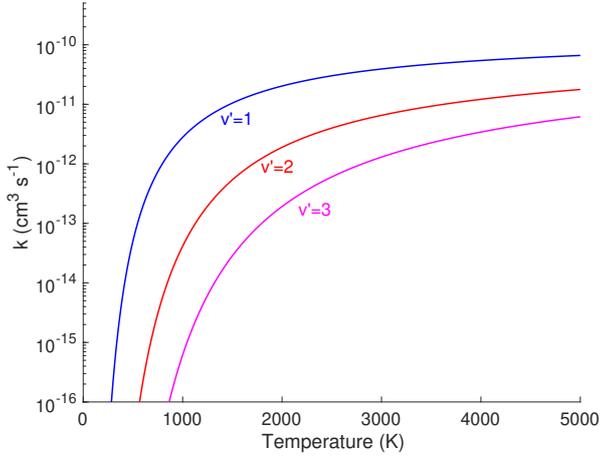
In Figure 2, we present the temperature variation of the state-to-state rate coefficients for the rotational de-excitation of HD by H from initial levels  $(v, j = 1)$  and  $(v, j = 2)$  to final level  $(v, j' = 0)$ . The most dominant transitions are those with  $\Delta j = 1$ . This is explained by the dominant odd anisotropy term of the HD-H PES as already discussed by Flower & Roueff (1999a) and Desrousseaux et al. (2018). For these transitions, at high temperature ( $T > 1000$  K), rate coefficients decrease with increasing HD initial vibrational state. Interestingly, the opposite behaviour is observed for transitions with  $\Delta j = 2$ .

The temperature dependence of the thermal rate coefficients for the vibrational excitation of HD induced by H is presented in Figure 3. These thermal rate coefficients were obtained by Boltzmann averaging using the partition function of the rotational states of the HD molecule in its ground vibrational state:

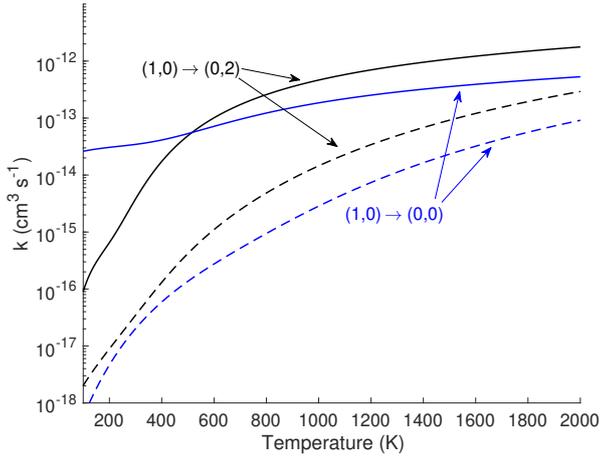
$$k_{v=0 \rightarrow v'} = \sum_j \sum_{j'} \frac{(2j+1) \cdot e^{-\frac{\epsilon_{v=0,j}}{k_B T}}}{Q} \cdot k_{v=0,j \rightarrow v',j'}, \quad (5)$$



**Figure 2.** Temperature variation of the state-to-state rate coefficients for the rotational de-excitation of HD by H from initial level  $(v, j = 1)$  to final level  $(v, j' = 0)$  (upper panel) and from initial level  $(v, j = 2)$  to final level  $(v, j' = 0)$  (lower panel).



**Figure 3.** Temperature dependence of the thermal rate coefficients for the vibrational excitation of HD by H from initial ground vibrational level  $v = 0$  to  $v'$ .



**Figure 4.** Comparison between excitation rate coefficients predicted by the present calculations (solid lines) and those of Flower & Roueff (1999b) (dashed lines) for the ro-vibrational de-excitation of HD by H from initial level  $(v, j)$  to final level  $(v', j')$ .

where  $Q = \sum_j (2j+1) \cdot e^{-\frac{\epsilon_{v=0,j}}{k_B T}}$  is the partition function and  $\epsilon_{v=0,j}$  is the energy of the  $v = 0$  rotational levels of HD.

As it can be seen, the magnitude of the rate coefficients decreases with increasing  $\Delta v = v' - v$  and the overall vibrational excitation is relatively slow compared to pure rotational excitation. Already observed for the H + D<sub>2</sub> (Lique & Faure 2012), D + H<sub>2</sub> (Cheikh Sid Ely et al. 2017), T + D<sub>2</sub> (Lique 2020), and D + T<sub>2</sub> (Lique 2020) systems, such behaviour can be attributed to the weak coupling between vibrational states (Lique & Spielfiedel 2007; Saidani et al. 2013).

In Figure 4, results obtained using three-dimensional reactive calculations are compared to the previous results obtained by Flower & Roueff (1999b) neglecting the reactive nature of the HD–H system. Differences as large as several orders of magnitude at low temperatures and up to approximately one order of magnitude at

higher temperatures exist between the two sets of data. In Figure 5, we go further into the comparison between excitation rate coefficients predicted by the present calculations and the results reported in Flower & Roueff (1999b). For all the possible HD( $v, j$ ) + H → HD( $v', j'$ ) + H transitions, we compare the rate coefficients at four different temperatures (500 K, 1000 K, 1500 K and 2000 K). As it can be seen, the most dominant transitions ( $k > 10^{-11}$  cm<sup>3</sup> s<sup>-1</sup>) correspond to the pure rotational ones. For these transitions, the agreement between the two sets of data is relatively good, with differences staying within a factor  $\sim 3$ . However, for the less dominant rate coefficients, which generally correspond to rovibrational transitions, differences up to at least 3 orders of magnitude can be observed at all explored temperatures. These differences increase with increasing initial vibrational level. Globally, rate coefficients from Flower & Roueff (1999b) are lower than the present results. Such finding is surprising as Flower & Roueff (1999b) did not consider the reactive channels in their calculations, suggesting that their rate coefficients would be overestimated compared to those computed in this work (especially at high temperatures where the H<sub>2</sub> formation is efficient). Two main reasons can then explain such differences: (i) the use of two different PESs, as described in Desrousseau et al. (2018), and (ii) the impact of the exchange process on the rovibrational excitation as discussed in Lique (2015a).

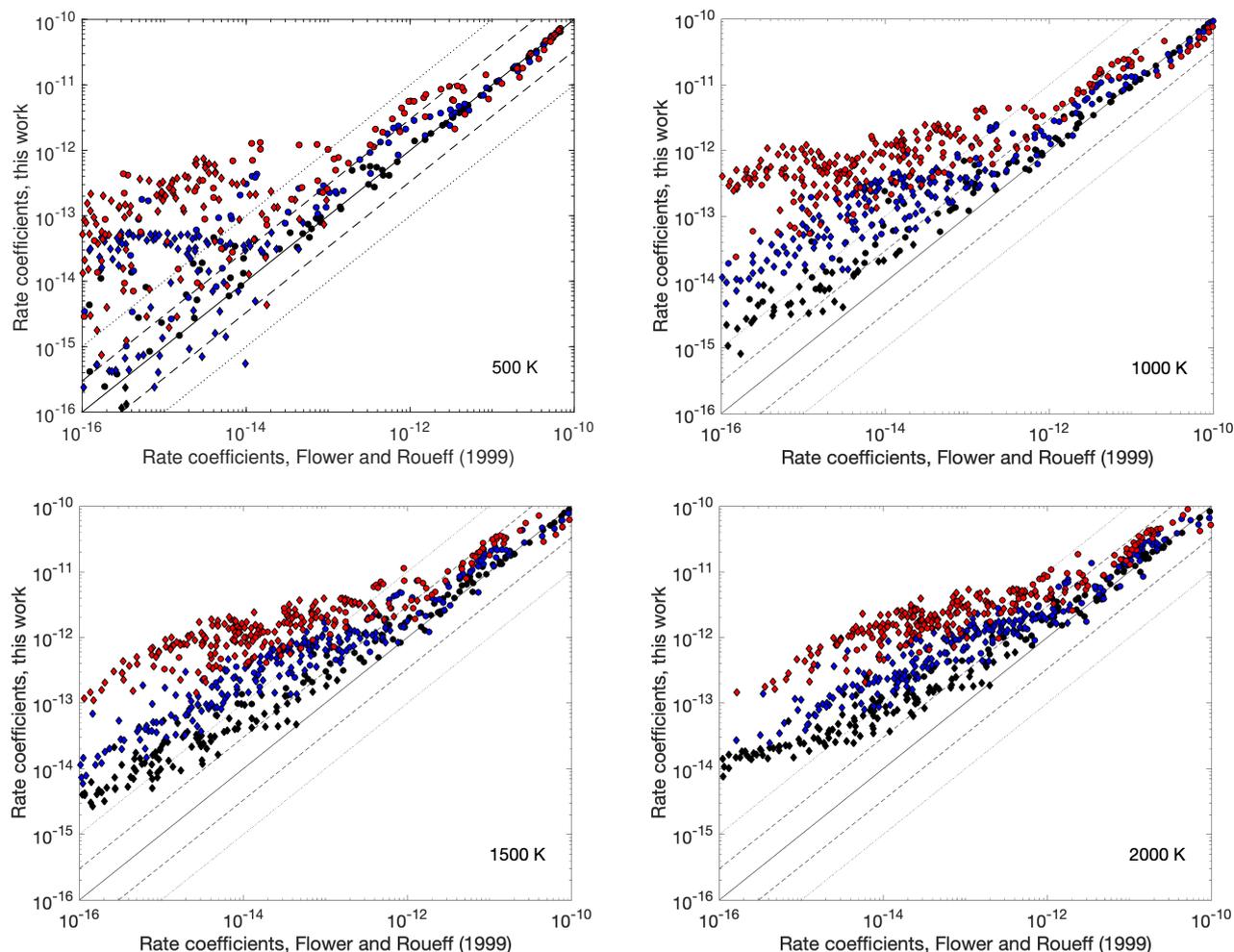
Rate coefficients presented by Zhou et al. (2021) for transitions between and within the  $v = 0$  and 1 vibrational levels and for temperatures ranging from  $T = 1 - 1000$  K (not shown on Figure 5) are in very good agreement with results obtained in the present work.

#### 4 SUMMARY AND CONCLUSIONS

Assuming LTE conditions often leads to an inaccurate description of astrophysical environments (Roueff & Lique 2013b). Hence, reliable state-to-state rate coefficients are an essential input to proceed in the description of the kinetics of level population in kinetic and radiative transfer models. The availability of such rate coefficients in extended temperature regimes is required to allow for the description of different astrophysical environments where thermal conditions might be drastically different.

To summarise, we have presented quantum-mechanical reactive scattering calculations to obtain rate coefficients for the collisional excitation of HD by H. Rate coefficients were obtained for temperatures up to 5000 K for transitions between all ro-vibrational levels of HD with internal energies lower than 14,000 cm<sup>-1</sup>. Results presented here have been compared to those by Flower & Roueff (1999b) where the exchange and reactive channels in the scattering calculations have been neglected. The comparison shows differences of a factor  $\sim 3$  for the most dominant transitions ( $k > 5 \times 10^{-12}$  cm<sup>3</sup> s<sup>-1</sup>). For the other transitions, differences up to several orders of magnitude can be seen at all temperatures explored in this work. As it has already been observed for several isotopic variants of the HD–H collisional systems (Lique & Faure 2012; Cheikh Sid Ely et al. 2017; Lique 2020), we also found that the vibrational excitation is slow compared to the pure rotational excitation.

The collisional rate coefficients presented in the present paper represent a big step in the complete description of the HD–H collisional system. Highly accurate collisional data for temperatures as high as 5000 K have been reported here, thus providing useful data to model a wide variety of astrophysical environments where the HD molecule is detected.



**Figure 5.** Comparison between excitation rate coefficients predicted by the present calculations and the results by Flower & Roueff (1999b) for all  $\text{HD}(v, j) + \text{H} \rightarrow \text{HD}(v', j') + \text{H}$  transitions at 500 K, 1000 K, 1500 K and 2000 K. The two dashed (dotted) lines delimit the region where the rate coefficients differ by less than a factor 3 (10). Rate coefficients for transitions from HD in its vibrational state  $v = 0, 1, 2$  are represented in black, blue, and red, respectively. Pure rotational transitions are represented with a circle symbol and transitions with a different final vibrational state are represented with a diamond symbol.

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## DATA AVAILABILITY

The data that support the findings of this study are available within the article and its online supplementary material.

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