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Collisional rate coefficients for astrophysics

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Abstract. In the interstellar medium, inelastic collisions are so rare that they cannot maintain a local thermodynamical equilibrium (LTE). Atomic and molecular populations therefore do not follow a simple Boltzmann distribution and non-LTE spectra are the rule rather than the exception. In such conditions, accurate state-to-state collisional data are crucial for a quantitative interpretation of spectra. In recent years, considerable progress has been made in quantum calculations of inelastic cross sections for a variety of targets, types of transitions and projectiles. For a few benchmark species, detailed comparisons between theory and experiment were also carried out at the state-to-state level and in the quantum regime. In this article, we highlight such comparisons for three important molecules: CO, H₂O and CH⁺. We also describe current computational efforts to extend these advances to ever larger targets, new transition types, and new environments (e.g. stellar envelopes or cometary atmospheres).

Keywords. Molecular data, molecular processes, scattering

1. Introduction

In the 1950s, and for many years before, astronomical spectroscopy was focused on the detection of atomic species. In 1956, however, Charlotte E. Moore proposed to extend laboratory works to molecular spectroscopy and she wrote that “The door is open and the opportunity is rich for the student interested in spectra. The more unusual examples of astrophysical identifications [...] all challenge the astrophysicist and in themselves more than justify active financial support of spectroscopic research in the laboratory, in theoretical fields, and in the observatory” (Moore 1956). Astronomical spectroscopy has made great strides over the past sixty years and a large variety of interstellar molecules have been discovered, but the above sentence is still relevant today.

To date, more than 270 gaseous molecular species (excluding isotopologues) have been identified in the interstellar medium (ISM) or in circumstellar envelopes[†]. Most of these molecules were detected in the microwave and (sub)millimeter ranges corresponding to rotational transitions. A handful of them were also detected as molecular ices *via* vibrational absorption transitions in the infrared. In the gas-phase, molecular lines can appear in emission or absorption, depending on the physical conditions along the lines of sight. The translation of the observed intensities to the molecular column density requires to understand the transfer of radiation within the astronomical source. This in turn requires access to spectroscopic data. In the microwave and (sub)millimeter ranges, spectroscopic data consist of line frequencies, line intensities and energy levels. In addition, because interstellar molecules are rarely at local thermodynamical equilibrium (LTE), a very good knowledge of inelastic collisional rate coefficients is necessary. Indeed, the frequency of inelastic collisions at interstellar densities is usually too low to maintain LTE so that the molecular excitation, i.e. the relative occupation of the energy levels, cannot be described

[†] <https://cdms.astro.uni-koeln.de/classic/molecules>

by a single “excitation temperature”. In such conditions, the quantitative analysis of a spectrum requires to solve simultaneously the (coupled) radiative transfer and statistical equilibrium equations.

In the present article, we discuss recent advances in the field of collisional excitation, focusing on rotational energy transfer between a molecule and H_2 or a free electron. In Section 2, we briefly present the theoretical and experimental methods available to study inelastic collisions at interstellar temperatures. In Section 3, three key molecules CO , H_2O and CH^+ are used as benchmark species to illustrate the good agreement achieved between theory and experiment at the state-to-state level and at very low energies. Section 4 describes current theoretical efforts to extend calculations to ever more challenging systems. A conclusion is given in Section 5.

2. Rotational energy transfer

2.1. Theory

At the low kinetic temperatures of interstellar clouds, the de Broglie wavelength of the abundant projectiles (H , He , H_2 and electrons) is comparable with or larger than the size of the target so that a quantum treatment of the collision dynamics is, in general, necessary. The quantum theory of rotational energy transfer between a rigid diatom and a spherical atom has been formulated in the late 1950s by Arthurs and Dalgarno (1960). It was generalized to polyatomics and open-shell diatomics (i.e with a fine structure) in the 1970s and 1980s (see e.g. Green & Thaddeus 1976 and Alexander & Dagdigian (1985)). The general formalism takes place within the Born-Oppenheimer approximation for the separation of the electronic and nuclear motions. The process consists of two steps: first, the electronic Schrödinger equation is solved using quantum chemistry methods, providing the so-called potential energy surface (PES). The nuclear motion over the (fitted) PES is solved separately, in a second step, using scattering methods. For the quantum chemistry part of the problem (first step), the coupled-clusters method (usually at the CCSD(T) level of theory) is known as the gold-standard because it is one of the most accurate methods applicable to medium-sized systems (i.e. up to 10-20 atoms with an accuracy of $\sim 1 \text{ cm}^{-1}$). For the scattering part (second step), the gold standard is the (time-independent) close-coupling or coupled-channel theory, which is the most accurate method but computationally prohibitive when the number of coupled channels N exceed $\sim 10,000$ †. Approximate methods include decoupling approximations (to reduce the number of coupled channels), statistical approximations and (time-dependent) classical or mixed quantum/classical approaches. More details about the theoretical methods can be found in the book edited by Lique and Faure (2019) (see dedicated Chapters 5 and 7).

We present in Fig. 1 an illustration of the convergence of scattering calculations as function of years for arguably the most studied collisional system: the rotational excitation of $\text{CO}(j \rightarrow j')$ by para- $\text{H}_2(j_2 = 0)$ (simply denoted as para- H_2 below). The rate coefficients for the two transitions $j = 0 \rightarrow 1$ and $j = 0 \rightarrow 2$ are found to vary within a factor of 2 since the 1970s before convergence to better than 5 percent is reached after 2010. The close-coupling method was used in all the listed references so that the observed convergence entirely reflects the increased accuracy of the $\text{CO}-\text{H}_2$ PES. Indeed, while the close-coupling method is an ‘exact’ method (provided the coupled channel basis set is complete), uncertainties in the PES has a significant impact on the scattering cross sections. We note that The development of more and more accurate PES coincides with

† The CPU time required by close-coupling calculations scale as N^3 and memory as N^2 .

advances in quantum chemistry but also with the massive increase in computational resources over the last two decades.

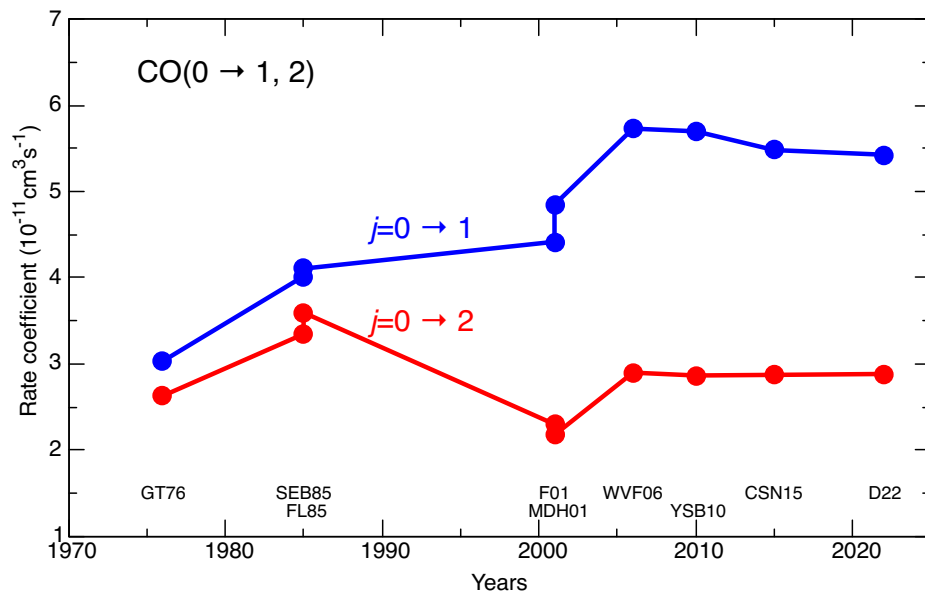


Figure 1. Theoretical rate coefficients for the rotational excitations $j = 0 \rightarrow 1, 2$ of CO due to para- H_2 as function of years. The kinetic temperature is 10 K. References are: Green and Thaddeus (1976) (GT1976), Schinke *et al.* (1985) (SEB1985), Flower and Launay (1985) (FL85), Flower (2001) (F01), Mengel, de Lucia, and Herbst (2001) (MHD01), Wernli *et al.* (2006) (WVF06), Yang *et al.* (2010b) (YSB10), Chefdeville *et al.* (2015) (CSN15), Dagdigian (2022) (D22).

2.2. Experiment

Recent experimental advances in the preparation of cold molecules ($\gtrsim 1$ K) have enabled the control of rotational states and have revealed quantum properties of molecular collisions, such as resonances and interferences. Neutral targets can be studied using crossed-molecular beam and flow-based methods while ions can be monitored in ion-trap and storage-ring apparatus. In recent years, these methods combined with laser techniques have been able to provide state-to-state data for molecular collisions of astrophysical interest. In particular, crossed-beam measurements can extract *relative* but *energy dependent* cross sections in a regime where resonances[†] can be observed. Because these resonances are extremely sensitive to small details in the interaction anisotropy, crossed-beam experiments provide a critical test of the PESs (see e.g. Shuai *et al.* (2020); Bergeat *et al.* 2020b). On the other hand, cold flow and ion-trap experiments can provide *absolute* and *temperature dependent* rate coefficients. Such measurements on an absolute scale provide another critical benchmarking of theory (e.g. Endres *et al.* 2021; Labiad *et al.* 2022). Careful and complementary experiments have thus become available to check

[†] A resonance is a sharp enhancement in the cross section when the collision energy matches the energy of a metastable state of the collision complex.

theoretical predictions in fine details, as illustrated below. For a recent review on experimental techniques, the reader is referred to Toscano, Lewandowski, and Heazlewood (2020).

3. Comparisons between theory and experiment

3.1. Carbon monoxide

Carbon monoxide (CO) is the second most abundant molecule in the ISM, after H₂. CO is the easiest molecular species to detect in galaxies, including high-redshift galaxies, and it is used to estimate masses of molecular clouds. It is also the second most abundant molecule in the coma of comets, after H₂O.

As illustrated in Fig.1, collisional excitation of CO by H₂ has been extensively studied theoretically in the past 50 years. In 2012, Chefdeville *et al.* (2012) have reported the first high-resolution state-to-state crossed-beam experiment on CO + para-H₂ using a variable crossing-angle. They were thus able to observe, for the first time, scattering resonances in an inelastic collision. Only qualitative agreement with theory was found but the authors later discovered an experimental bias in their treatment and corrected data were then published in Chefdeville *et al.* (2015). These corrected data are presented in Fig. 2 for the excitation CO($j = 0 \rightarrow 1$) by normal-H₂. The agreement with theory is very good, almost within error bars, with the position and amplitude of the three resolved 'bumps' (at $\sim 7, 12$ and 18 cm^{-1}) nicely reproduced by the convoluted theory.

Very recently, the same system CO + H₂ was measured in cold supersonic flows by Labiad *et al.* (2022). State-to-state rate coefficients were reported for CO($j_i = 0, 1, 4$) and kinetic temperatures in the range 5–20 K. A sample of measured data are presented in Fig. 3 for CO excitations $j = 0 \rightarrow 1 - 4$ at $T_k = 20$ K. Agreement with theory is again very good. In particular, the rate coefficient for $j = 0 \rightarrow 2$ is found to be larger than that for $j = 0 \rightarrow 1$, reflecting the well-known $\Delta j = 2$ propensity rule in almost homonuclear molecules. This propensity is due to quantum mechanical (interference) effects related to the even anisotropy of the CO–H₂ PES. From the whole set of experimental data, the agreement with theory was found to be typically within 20 %.

3.2. Water

Water is ubiquitous in the Universe and it is the third most abundant molecule, after H₂ and CO. Many rotational transitions can be detected in the ISM, including masers, and a rich ro-vibrational spectrum is observed in evolved stars. Water is also the dominant component of interstellar and cometary ices.

The excitation of H₂O was revisited theoretically in the 2000s during the scientific preparation of the Herschel Space Observatory (see van Dishoeck, Herbst, and Neufeld (2013) and references therein). Experimentally, the first state-to-state (differential) measurements for H₂O+para-H₂ were performed in a crossed-beam apparatus at high collision energy ($\sim 500 \text{ cm}^{-1}$) by Yang *et al.* (2010a). The cold regime was investigated more recently by Bergeat *et al.*(2020a) for the collisions between H₂O and normal-H₂. Integral cross-sections were measured but resonances were too weak to be detected. Heavy water (D₂O) was used in a subsequent study with para-H₂ as the projectile Bergeat *et al.* 2020b. Indeed, theory has predicted resonances to be much easier to detect with para-H₂ than with normal-H₂, thanks to the smaller number of overlapping resonant features. In addition, the use of D₂O rather than H₂O substantially reduces the background signal and thus improves the signal-to-noise ratio. The cross section for the transition D₂O($0_{00} \rightarrow 2_{02}$) due to para-H₂ is shown in Fig. 4. As for CO + H₂, excellent agreement between theory and experiment is observed. In particular, four bumps are resolved (at

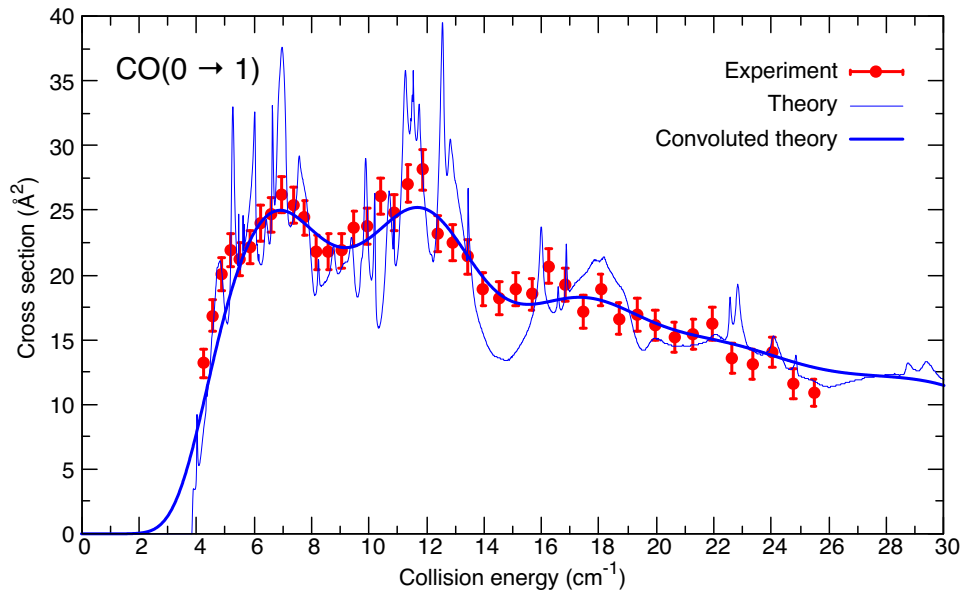


Figure 2. Comparison of experimental and theoretical cross sections for the CO excitation $j = 0 \rightarrow 1$ by normal- H_2 as function of the collisional energy. The thin solid line gives the pure theoretical cross sections while the thick solid line denotes the same theoretical data convoluted with the experimental energy spread. Experimental data (red circles) have been normalized to the convoluted theoretical cross sections. Experimental errors correspond to 2σ . Adapted from Chefdeville *et al.* (2015).

$\sim 37, 46, 55$ and 68 cm^{-1}) and they are perfectly reproduced by convoluted theory, both in absolute positions and relative intensities. We note that the signal below threshold (at 35.9 cm^{-1}) is due to both the presence of some $\text{D}_2\text{O}(1_{11})$ in the beam and the contribution from the 2_{12} level in the REMPI signal (see Bergeat *et al.* (2020b)). A detailed partial-wave analysis was also presented in Bergeat *et al.* (2020b) where full details can be found.

3.3. Methylidinium

Methylidinium (CH^+) was among the first three interstellar molecules detected in absorption toward bright stars, in the early 1940s. It is a good tracer of warm interstellar regions, where endothermic reactions can occur, but its high abundance in the diffuse ISM is a long standing, still debated, puzzle Godard *et al.* 2022.

The excitation of CH^+ in the ISM is a difficult problem because this ion reacts quickly with the most abundant colliders, i.e. H , H_2 and electrons. It thus belongs to the class of “reactive species” for which destruction channels compete with inelastic (including exchange) channels. Such species can thus not fully equilibrate through inelastic collisions. Models of CH^+ excitation can be found in Godard and Cernicharo (2013) and Faure *et al.* (2017). Experimentally, state-to-state measurements for $\text{CH}^+ + \text{e}^-$ were carried out very recently in the cryogenic storage ring (CSR) in Heidelberg. By combining laser probing of CH^+ rotational states j with a merged electron beam, Kálosi *et al.* (2022) were able to extract a cross-section for the ground-state excitation $j = 0 \rightarrow 1$. The corresponding rate

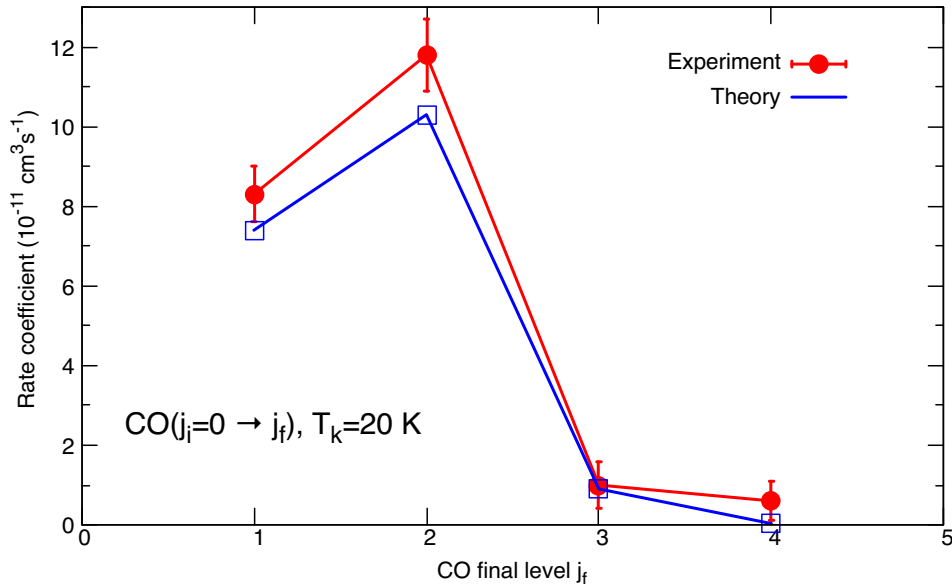


Figure 3. Comparison of experimental (red circles) and theoretical (blue squares) state-to-state rate coefficients for the CO excitations $j = 0 \rightarrow 1 - 4$ at 20 K. Experimental errors correspond to 2σ . Adapted from Labiad *et al.* (2022).

coefficient is plotted in Fig. 5 and is compared to the theoretical calculations of Hamilton, Faure, and Tennyson (2016) based the R -matrix method. Theory lies within the experimental uncertainty ($\pm 43\%$) with an agreement better than 30%. We note that the R -matrix calculations employ the Coulomb-Born approximation to include long-range effects due to the substantial CH^+ dipole (1.7 D).

4. Perspectives

The results presented in Section 3 were limited to rotational energy transfer between small molecules (with 2 or 3 atoms) and H_2 or a free electron. For such relatively small collisional systems, state-of-art experimental measurements have confirmed that quantum scattering theory has reached a high degree of predictability and that great confidence can be placed in recent (i.e. past 10-20 years) theoretical state-to-state rate coefficients. As explained above, the key ingredient in these calculations is the PES, especially if the kinetic temperature is low. High-accuracy PESs can be determined for larger systems (including up to ~ 20 atoms) and the main computational limit is thus the number of coupled channels in the close-coupling equations. We describe below new perspectives and methods to overcome the current challenges.

4.1. Large molecules and heavy projectiles

Close-coupling calculations become computationally challenging for molecules with typically more than 6 atoms, and recent studies have indeed employed the He atom as a substitute for H_2 in order to reduce the computational cost, for example in the case of

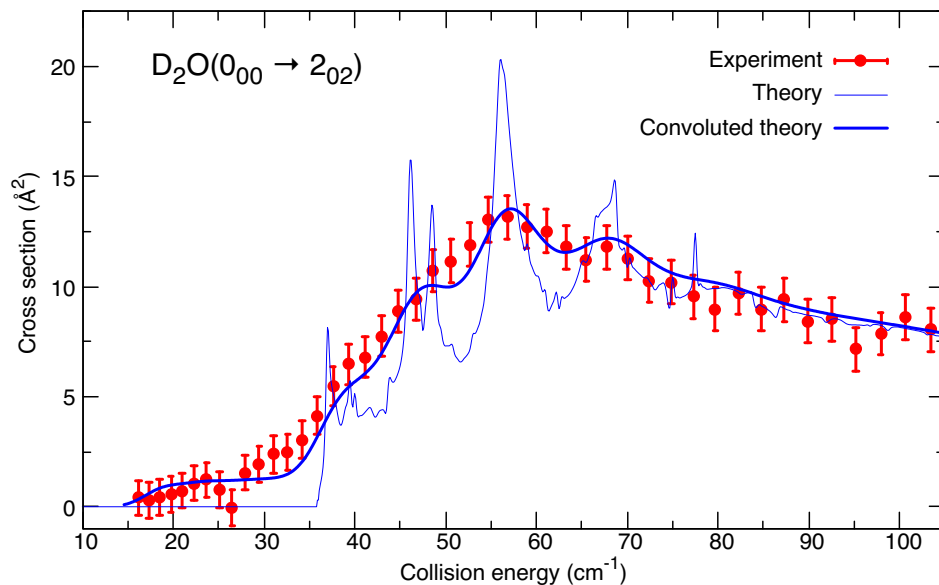


Figure 4. Comparison of experimental and theoretical cross sections for the $\text{D}_2\text{O}(0_{00} \rightarrow 2_{02})$ by para- $\text{H}_2(j_2 = 0)$ as function of the collisional energy. The thin solid line gives the pure theoretical cross sections while the thick solid line denotes the same theoretical data convoluted with the experimental energy spread. Experimental data (red circles) have been normalized to the convoluted theoretical cross sections. Experimental errors correspond to 2σ . Adapted from Bergeat *et al.* (2020b).

the ten-atom species $\text{CH}_3\text{CHCH}_2\text{O}$ (chiral propylene oxide) (Faure *et al.* 2019). For even larger molecules, with more than 12 atoms, approximate dynamical methods become necessary. For example, the mixed quantum/classical theory (MQCT) was used recently to compute the rotational (de)excitation of benzene (C_6H_6) by He atoms (Mandal *et al.* 2022). In addition to the target, the projectile also can bring complexity. Thus, in the case of collisions with H_2O or CO , which are the dominant colliders in cometary atmospheres, the number of coupled channels exceeds the computational limits for the very lowest partial-waves so that it is currently not possible to compute a fully converged close-coupling rotational cross section, even at very low energy. Besides MQCT, the coupled-state (CS) decoupling approximation and the statistical adiabatic channel model (SACM) are possible alternatives, as employed respectively for $\text{HCN} + \text{H}_2\text{O}$ (Dubernet & Quintas-Sánchez 2019) and $\text{CO} + \text{H}_2\text{O}$ (Faure *et al.* 2020). Benchmarking calculations comparing these different methods would be of great interest.

4.2. Vibrational excitation

Including the vibrational degrees-of-freedom is also very demanding, even for small molecules, because vibrational excitation involve higher temperatures and thus more coupled channels. Thus, in practice, available ro-vibrational state-to-state collisional data are almost exclusively restricted to diatomic targets (e.g. Yang *et al.* 2015). Vibrational studies on polyatomic targets are scarce but recent developments can be found in the works of Stoecklin *et al.* (2019) and Wiesenfeld (2021) on $\text{H}_2\text{O} + \text{H}_2$, Selim, van der Avoird, and

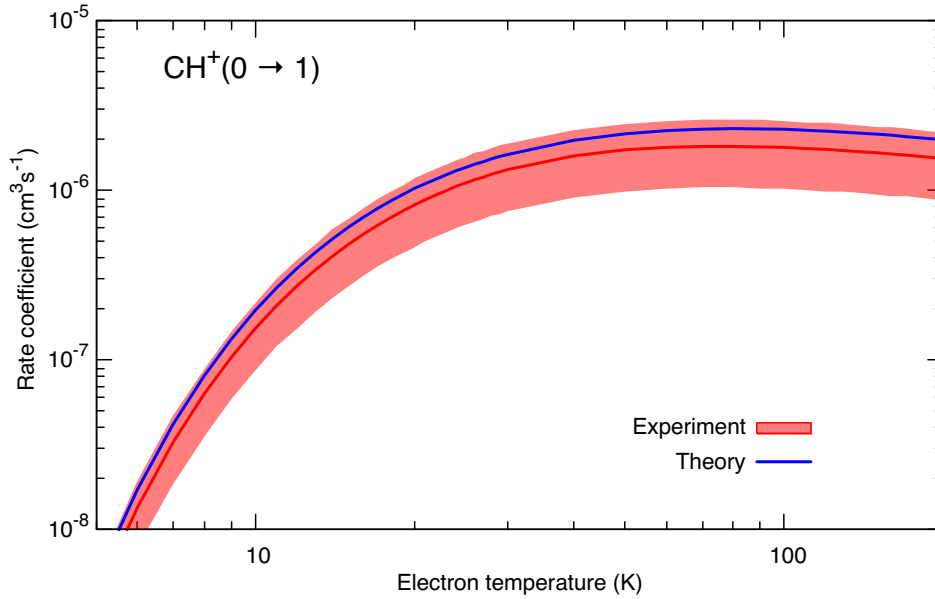


Figure 5. Comparison of experimental (red line and shaded 1σ uncertainty) and theoretical (blue line) rate coefficient for the CH^+ excitation $j = 0 \rightarrow 1$ as function of electron temperature. Adapted from Kálosi *et al.* (2022).

Groenenboom (2022) on $\text{CO}_2 + \text{He}$ and Ayouz *et al.* (2021) on $\text{H}_2\text{O} + \text{e}^-$. The knowledge of ro-vibrational data is important to model molecules such as water in hot stellar envelopes but also for molecules that are not accessible through rotational transitions, e.g. H_2 , CH_4 , CO_2 , etc. to be observed with the recently launched infrared James Webb space telescope (JWST). Ro-vibrational data are also required for larger and floppier molecules with low-frequency modes (e.g. internal rotations) which can be excited even at relatively low temperatures. We note in this context that only the torsional excitation of methanol by He atoms has been investigated (Rabli & Flower (2011)).

4.3. Excitation of atoms

The electronic excitation of atoms by H was also revisited in the last decade. Inelastic collisions with electrons and hydrogen atoms are important to model non-LTE atomic spectra in cold stellar atmospheres. Accurate theoretical rate coefficients are now becoming available for atoms such as MgI, CaI and OI (see Belyaev *et al.* 2019 and references therein).

4.4. Reactive species

Finally, for reactive species such as CH^+ where the inelastic and reactive channels are in competition, statistical methods provide a useful and efficient approach. For example, the SACM and statistical quantum mechanical (SQM) methods were employed successfully to treat triatomic reactive systems, see e.g. the recent works of González-Lezana, Hily-Blant, and Faure (2021) and Konings *et al.* (2021). More generally, statistical methods apply to PESs with a deep well where a long-lived intermediate complex can form,

resulting in a statistical redistribution of the product energy levels (see Dagdigian 2017). Their accuracy in favorable cases is better than 50% at the state-to-state level. Their extension to polyatomic targets is underway (Lique, Loreau and co-workers) and should allow to consider polyatomic molecular ions such as H_2O^+ colliding with H or H_2 .

5. Conclusions

The last two decades have seen an impressive improvement of inelastic scattering calculations, thanks to progress both in quantum chemistry and computational resources. Spectacular agreements between theory and experiment have also confirmed the good accuracy ($\pm 25\%$) of collisional cross sections and rate coefficient. Collisional data are compiled in dedicated databases such as LAMDA in Leiden (van der Tak et al. 2020), BASECOL in Paris (Ba et al. 2020) and the more recent EMAA database in Grenoble. Current challenges are numerous and difficult, and include heavier targets and projectiles, higher temperatures and reactive species. To paraphrase Charlotte E. Moore, the door is open and the opportunity is rich for the student interested in collisions.

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