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Electron fraction and the excitation of interstellar HCO^+

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Abstract. In the most energetic regions of space (shocks, photodissociation regions, etc.), the electron fraction, x_e, can increase by several orders of magnitude. When x_e exceeds about 10^{-5}, free electrons can compete or even dominate over neutrals in the excitation of molecules. Recent theoretical studies, based on the molecular **R**-matrix method, have revisited the electron-impact excitation of many interstellar molecules. We focus in this paper on the rotational excitation of the $H^{13}CO^+$ molecular ion which was recently detected towards a molecular cloud exposed to ionizing cosmic rays. We present results from non-LTE radiative transfer calculations and we show that the physical conditions inferred from the observations are consistent with an electron density enhancement ($x_e > 10^{-6}$) if the column density of the ion is below $\sim 6 \times 10^{12}$ cm^{-2}.

Key words. molecular data – molecular processes – plasmas – ISM: molecules

1. Introduction

Cosmic rays (CRs) are a primary source of ionization in the interstellar medium (ISM), competing with UV and X stellar photons. The electron or ionization fraction, $x_e = n_e/n_H$, is a crucial parameter that controls both the coupling of the gas with the galatic magnetic field and the formation/destruction of molecules, which contribute to the energy loss of the molecular clouds. CRs also produce heating because the $\sim$ 30 eV energy of the secondary electrons produced by the ionization of H_2 (Cravens & Dalgarno 1978) is partly converted into heat through inelastic collisions with atoms and molecules. A discussion on the thermalization of electrons in the ISM can be found in Field et al. (2007).

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The abundance of free electrons in the ISM is difficult to measure with precision. In dark molecular clouds, it is usually estimated by measuring the degree of deuterium fractionation (see e.g. Caselli et al. 1998, and references therein). In these environments, the electron fraction is typically below 10^{-6}. In regions where the fraction exceeds $\sim 10^{-5}$, the non-local thermodynamic equilibrium (LTE) excitation of molecules can also be used as a probe of the electron abundance. Indeed, at such fractions, free electrons are expected to drive the molecular excitation because rate coefficients for electron-impact excitation are typically 4-5 orders of magnitude greater than the corresponding rates for excitation by neutrals (He, H and H_2). The first evidence for an electron density enhancement in a C-type shock was thus provided by the observation of an overexcitation of $H^{13}CO^+$ towards the

L1448-mm outflow (Jiménez-Serra et al. 2006; Roberts et al. 2010). Molecular ions with large dipoles are the most sensitive tracers of the electron-impact excitation, as explained in Jiménez-Serra et al. (2006). Other sources with high electron fraction include diffuse molecular clouds, photon-dominated regions (PDRs), X-ray dominated regions (XDRs) and cosmic ray dominated regions (CRDRs).

In this paper, we discuss the recent detection of $H^{13}CO^+$ towards a molecular cloud exposed to ionizing CRs (Ceccarelli et al. 2011). As in Jiménez-Serra et al. (2006), electron-impact excitation rates are used to determine the ionization fraction which, in turn, can be employed to infer the (controversial) CR ionization rate. The next section briefly presents the theoretical excitation rates for HCO^+. Non-LTE radiative transfer calculations are compared to observational data in Section 3. Conclusions are drawn in Section 4.

2. Excitation rates for HCO^+

The reference method for computing electron-impact excitation rates for molecular ions has been the Coulomb-Born (CB) approximation. This approach assumes that the excitation rates are entirely determined by long-range interactions. A standard further approximation is to consider only the dominant long-range term. Within this model, only single jumps in rotational quanta ($\Delta J = 1$) are allowed for polar species. Recent **R**-matrix calculations combined with the adiabatic-nuclei-rotation (ANR) approximation have been applied to various ions and have shown that the inclusion of short-range interactions actually lead to significant rates for dipole forbidden transitions (Faure & Tennyson 2001; Faure et al. 2006). On the other hand, the collisional propensity rules were generally found to be consistent with the CB theory. As a result, dipole-allowed transitions are always preferred for highly polar ions like HCO^+. The accuracy of the **R**-matrix/ANR approach has been confirmed recently by comparing theoretical and experimental rate coefficients for inelastic collisions of HD^+ with cold electrons (Shafir et al. 2009). The validity of the ANR approximation down to very low energy was also demonstrated theoretically in Faure et al. (2006). A recent review of the UK molecular **R**-matrix method and its recent applications can be found in Tennyson (2010).

Electron-impact excitation rates for HCO^+ were first computed by Faure & Tennyson (2001). These rates were then extended to lower temperatures and higher angular momenta in Jiménez-Serra et al. (2006), where details can be found. An overall presentation of the HCO^+ rates at 20 K is given in Fig. 1. In this plot, the electron-impact rates are plotted versus the corresponding para-H_2 rates. The HCO^+-H_2 rates were taken from Flower (1999). It can be first observed that the largest electron-impact rates exceed those for H_2 by 4-5 orders of magnitude, as expected. These rates correspond to dipole allowed ($\Delta J = 1$) transitions. We also notice that there is a large dispersion of the electron-impact rates and that for some transitions ($\Delta J > 6$), HCO^+-H_2 rates are in fact larger than those for electron-impact.

3. HCO^+ excitation towards W51 C

The recent detection of $H^{13}CO^+$ towards a molecular cloud associated with the supernova remnant (SNR) W51 C (Ceccarelli et al. 2011) provides a potential interesting application to study electron-impact excitation. W51 C is indeed one of the most luminous γ-ray sources of our galaxy. A strong electron density enhancement is therefore expected within the associated molecular cloud. Ceccarelli et al. (2011) have employed the observed $[DCO^+]/[H^{13}CO^+]$ ratios to measure the gas ionisation degree of the cloud. A large value, $x_e \gtrsim 2 \times 10^{-5}$, was thus analytically derived toward a particular position in the cloud. High values of x_e were also obtained by a detailed chemical modelling from which the authors have determined a CR ionization rate $\zeta \sim 1.4 \times 10^{-15} s^{-1}$, i.e. enhanced by two orders of magnitude with respect to the standard value. While the general conclusion of an electron density enhancement is certainly robust, the estimation of x_e from the $[DCO^+]/[H^{13}CO^+]$ ratio is not straightforward and rather uncertain.

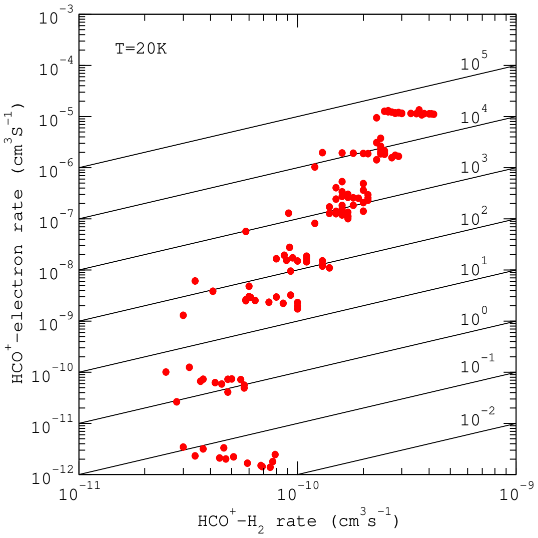

Fig. 1. Comparison between the rate coefficients for rotational excitation of HCO^+ by electron-impact and H_2 collisions. Deexcitation transition rates are reported for the lowest 21 rotational levels at 20 K. The horizontal axis represents the para-H_2 rates (in units of $cm^3 s^{-1}$) of Flower (1999) and the vertical axis represents the corresponding electron-impact rates of Faure & Tennyson. The solid lines represent the scaling factors between the two axes. See text for details.

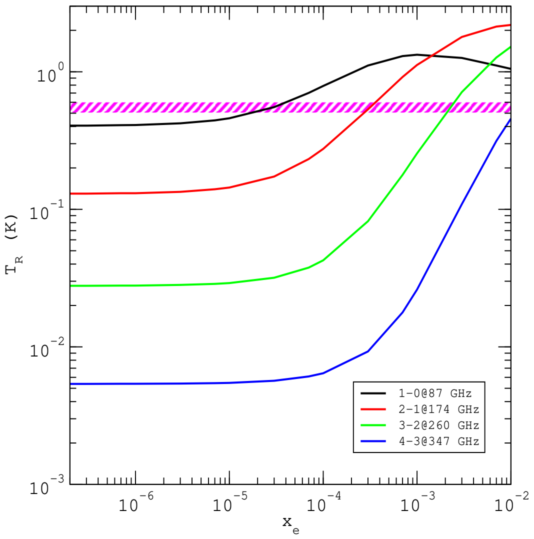

Fig. 2. Radiation peak temperature, T_R (in Kelvin), for the four lowest transitions of $H^{13}CO^+$ as a function of the electron fraction. Peak intensities were computed with the RADEX code. The observed intensity towards W51 C for the $1 \rightarrow 0$ line at 87 GHz (Ceccarelli et al. 2011) is given by the hashed area. See text for details.

In this section, we examine the influence of the electron fraction x_e on the $H^{13}CO^+$ emission using non-LTE radiative transfer calculations. Collisional excitation by free electrons and para-H_2 molecules is considered. The de-excitation rates of Flower (1999) for HCO^+-H_2 are employed for the ^{13}C isotopologue. Electron-impact excitation rates are taken from Jiménez-Serra et al. (2006). Energy levels and Einstein radiative coefficients were taken form the LAMDA database[1]. Radiative transfer calculations were performed with the `RADEX` code (van der Tak et al. 2007), using the Large Velocity Gradient (LVG) approximation for an expanding sphere. The temperature and H_2 density were fixed at the values determined by Ceccarelli et al. (2011), i.e. T=20 K and $n(H_2) = 10^4 cm^{-3}$. The line width was taken to be 3 kms^{-1}, as observed. The column density was fixed at $N(H^{13}CO^+) = 4 \times 10^{12} cm^{-2}$ and only the electron abundance was varied from 10^{-3} to 10^2 cm^{-3}, corresponding to electron fractions in the range 10^{-7} to 10^{-2}. Results are presented in Fig. 2. It can be observed that there is a significant increase of all line intensities when x_e exceeds $\sim 10^{-5}$, as expected. In particular, we note that the intensity of the $1 \rightarrow 0$ transition at 87 GHz, as observed by Ceccarelli et al. (2011), can be reproduced for $x_e \sim 3 \times 10^{-5}$. Of course this value strongly depends on the assumed column density since in the optically thin regime, the peak intensity varies linearly with the column density. As a result, the detection of additional $H^{13}CO^+$ lines, e.g. at 174 and 260 GHz, would greatly help to constrain the column density and electron fraction. In any case, the present simulation provides a support for an electron density enhancement ($x_e > 10^{-6}$) if the column density of $H^{13}CO^+$ does not exceed $\sim 6 \times 10^{12}$ cm^{-2}.

4. Conclusions

We have investigated in this paper the excitation of the $H^{13}CO^+$ molecular ion in the conditions of a molecular cloud exposed to ionizing CRs. We have shown that electron-impact excitation can be employed to determine the electron fraction in such environments, provided that the ion column density is well constrained. In the present case of W51 C, the observation of Ceccarelli et al. (2011) is consistent with an electron density enhancement ($x_e > 10^{-6}$) if the column density is below $\sim 6 \times 10^{12}$ cm^{-2}. Electron-impact excitation rates are now available for a large number of charged and neutral molecules (see references in Tennyson 2010) and we strongly recommend to use these rates in any detailed non-LTE excitation model of ionized environments.

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[1] `http://www.strw.leidenuniv.nl/~{}moldata/HCO+.html`