Mem. S.A.It. Vol. 82, 925

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The influence of cosmic rays in PDR models applied to diffuse clouds

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Abstract. In diffuse interstellar gas, the formation of several key species is initiated by cosmic rays. In the last decades, several methods, based on the observation of these key species, have been used to infer the flux of cosmic rays. The discovery of H_3^+ towards ζ Perseus by McCall et al. (2003) suggested that the flux of cosmic rays can be higher by an order of magnitude than canonical value deduced from OH observations (10^{-17} s^{-1}). The discovery of H_3^+ in the center molecular zone also shows that a strong ionizing flux is present in this region. Recent discoveries by Herschel of OH^+ and H_2O^+ in spiral arms of the Galaxy confirm a high flux of cosmic rays. In this paper, we summarize these discoveries that force us to review the value of the flux of cosmic rays in the diffuse interstellar medium.

Key words. ISM: cosmic rays – ISM: molecules, ISM: general

1. Introduction

By partially ionizing the gas, cosmic rays allow ion-neutral reactions to take place. Such reactions are efficient since, in most of cases, they do not have energy thresholds and are fast compared to neutral-neutral reactions. It is well known, that, in dark clouds, without cosmic rays, chemical reactions could not take place (or at least on much longer time-scales). In diffuse clouds, even if the chemistry is strongly controlled by the external UV radiation field, the formation rate of several key species as OH, HD, H_3^+, ... is directly linked to the flux of cosmic rays. It is then important to be able to constrain this flux. In the field of interstellar chemistry, the flux of cosmic rays, ζ, is traditionally measured as the number of ionization of H_2 by cosmic rays per second. In this paper, we will present some elements of this field of study for diffuse clouds.

2. The Meudon PDR code

Detailed modeling of the physics and chemistry of the interstellar medium are done thanks to Photo-Dominated Regions (PDR) codes (see Röllig et al. (2007) for a review). Results presented in this paper have been obtained thanks to the Meudon PDR code (Le Petit, F. et al. 2006). The code computes the stationary atomic and molecular structure of a plane-parallel slab of dust and gas illuminated by an external radiation field. It solves consistently the radiative transfer, thermal balance and chemistry. The radiative transfer equation is solved from the far UV to the sub-millimeter domain. Absorption in the continuum by dust and in the lines of molecules is taken into

Send offprint requests to: F. Le Petit account. Thermal balance is solved assuming that the heating rate equals the cooling rate. Heating mechanisms taken into account are the photo-electric effect on grains, cosmic rays ionization, exothermic chemical reactions, etc. Cooling is due to emission in the lines of atoms and molecules. Because interstellar clouds are far from thermodynamical equilibrium, this requires to compute explicitly level populations of the main coolants. Chemistry takes into account several hundreds species linked by a network of several thousands reactions. Cosmic rays participates to the heating mechanisms (a minor process in front of photo-electric effect in diffuse clouds) and to the chemistry as we will see below. They are also responsible for the production of secondary UV photons.

After a run of the model, the code provides lines intensities and column densities that can be compared to observations. The code is public and can be downloaded on the web site : pdr.obspm.fr

3. The zeta Perseus line of sight

The assessment of the flux of cosmic rays in diffuse interstellar clouds has a long history. The 2 molecules initially used in this way have been OH and HD. In the case of OH, the ionization of atomic hydrogen by cosmic rays initiates a chain of charge exchange reactions that ends by a dissociative recombination with an electron :

$$\begin{aligned} \mathrm{H} + \text{cosmic ray} &\longrightarrow \mathrm{H}^+ + e^- \\ \mathrm{H}^+ + \mathrm{O} &\longrightarrow \mathrm{O}^+ + \mathrm{H} \\ \mathrm{O}^+ + \mathrm{H}_2 &\longrightarrow \mathrm{OH}^+ + \mathrm{H} \\ \mathrm{OH}^+ + \mathrm{H}_2 &\longrightarrow \mathrm{H}_2\mathrm{O}^+ + \mathrm{H} \\ \mathrm{H}_2\mathrm{O}^+ + \mathrm{H}_2 &\longrightarrow \mathrm{H}_3\mathrm{O}^+ + \mathrm{H} \\ \mathrm{H}_3\mathrm{O}^+ + e^- &\longrightarrow \mathrm{OH} + ... \end{aligned}$$

Federman et al. (1996) provide expressions of the relationships between n(OH) and n(HD) with ζ. The abundance of OH is directly proportional to ζ and to the elementary abundance of oxygen. Since the ratio O/H seems to be constant in the local interstellar medium (Meyer et al. 1998), it is straightforward to deduce ζ from the observation of OH. The situation is the same for HD (Le Petit et al. 2002) excepted that its elementary abundance is less well constrained than O/H (Hebrard & Moos 2003; Linsky et al. 2006).

That is the reason why OH observations on diffuse lines of sight have initially been one of the most direct way to infer the flux of cosmic rays (Black & Dalgarno 1973; Black & al. 1978; Federman et al. 1996). They found a mean value $\zeta \simeq 10^{-17}$ s^{-1} that became a canonical value. This value prevailed until the discovery of H_3^+ in the diffuse gas towards ζ Perseus by McCall et al. (2003). The formation of H_3^+ is also initiated by cosmic rays :

$$\begin{aligned} \mathrm{H}_2 + \text{cosmic ray} &\longrightarrow \mathrm{H}_2^+ + e^- \\ \mathrm{H}_2^+ + \mathrm{H}_2 &\longrightarrow \mathrm{H}_3^+ + \mathrm{H} \end{aligned}$$

The main destruction path of H_3^+ in diffuse clouds is the dissociative recombination with electrons. The discovery of H_3^+ on the line of sight towards ζ Per with a column density of $8{\times}10^{13}$ cm^{-2} led McCall et al. to review the canonical of ζ to a value about 100 times higher than the canonical value (10^{-15} s^{-1}). This was a surprise since ζ Perseus was one of the lines of sight used to infer the previous "canonical" value.
This work has been reviewed by LePetit et al. (2004) who did a comprehensive model of the ζ Perseus line of sight reproducing the column densities of all observed molecules. They took into account several parameters as the clumpiness of the medium and the gas temperature : some key reactions are highly dependent on it, as the charge exchange reaction between O and H^+. They also re-analyzed the data that permitted to deduce the column density of HD (Snow 1977). They showed that the observation of H_3^+ as well as the other species can be roughly reproduced (i.e. taking into account the error bars on the observations and the simplifications of the numerical models) with $\zeta = 2.5 \times 10^{-16}$ s^{-1}, lower than the value of McCall et al. (2004), obtained from the sole analysis of H_3^+. They showed that a higher flux of cosmic rays significantly overestimates column densities of some species. In diffuse clouds, the electron abundance is usually controlled by the ionization of carbon atoms by UV photons. If the ionization

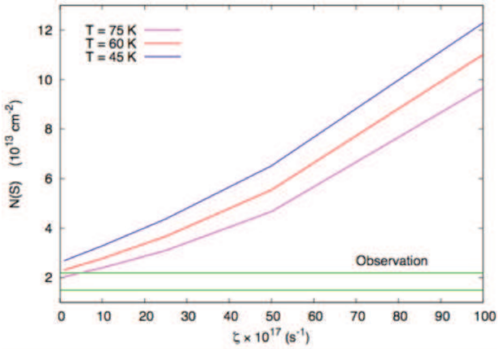

Fig. 1. Column density of S obtained for different values of ζ with the PDR code and the parameters of the ζ Per line of sight presented in Le Petit et al. (2004).

by cosmic rays is high, then the abundance of electrons can be increased and recombination of ionized species occurs more often producing to much of neutral species such as C or S. Fig 1 presents the column density obtained by models for different values of ζ. For $\zeta \simeq 10^{-15}$ s−1, the column density of neutral sulfur is overestimated by a factor 10. Moreover, with high flux of cosmic rays too high, the formation rate of OH is too much enhanced. This is even more the case if turbulence effect is also taken into account to explain n(CH^+) since this process also increases OH formation rate. Nevertheless, the detection of H_3^+ towards ζ Perseus by McCall et al. (2003) clearly showed that the flux of cosmic rays is significantly higher than the canonical value used from the 70s. The comprehensive model by LePetit et al. (2004) demonstrated that the inferring of the value of ζ has to be done taking into account all the constraints and not only one species.

4. The Galactic center

One interesting discovery of these past years has been the detection of H_3^+ towards the central molecular zone, CMZ, (Oka et al. 2005; Goto et al. 2008; Geballe & Oka 2010; Goto et al. 2011) in its levels (1,1), (2,2) and (3,3). Level (3,3) is metastable and its observation can provide informations on the density of the medium. Thanks to this detection, Oka et al. (2005) claimed to have discovered warm and diffuse clouds in the Galactic center.

We implemented the computation of the excitation of H_3^+ in the PDR code. Levels energies and radiative transitions data come from Miller & Tennyson (1988), and Lindsay & McCall (2001). Oka & Epp (2004) provide simple expressions for collision rates of H_3^+ with H_2. More precise data have been determined at T < 50 K by Hugo et al. (2009). They show the existence of selection rules not taken into account by Oka & Epp. Proper modeling requires collision rates at higher temperatures so we use a modified version of the formalism by Oka & Epp (2004) that aims at avoiding numerical difficulties that their exponential term could create in a code solving thermal balance.

Our computations show that the observed ratios (3,3)/(2,2) $\simeq$ 5 and (3,3,)/(1,1) $\simeq$ 1 can be reproduced in a medium at several 100 K and with a low density, $n_H \simeq 20$ cm^{-3}. This in relatively good agreement with the conclusions of Oka & Epp even if they concluded to a density around 50 cm^{-3}. This small difference come from the difference in the H_2 + H_3^+ collision rates. Interpretation of such observations would benefit from an extension of the computations of collision rates to higher temperatures than Hugo et al. works.

The column density of H_3^+ can be reproduced with a high ionizing rate. The sole observation of H_3^+ and the lack of knowledge of the UV flux makes difficult to quantify it precisely. Moreover, in the CMZ, this ionizing flux can be due to cosmic rays or X-rays. Our computation showed also that the ratios of level populations (3,3)/(2,2) is insensitive to ζ.

If these observations show all the interest to observe H_3^+ to deduce the properties of diffuse gas, in a so complex region, they have to be completed by observations of other species to be interpreted properly and to discriminate between cosmic and X rays.

5. Herschel discoveries

Herschel space telescope detected OH^+ and H_2O^+ in diffuse lines of sight (Gerin et al. 2010; Neufeld et al. 2010). As seen in section 3, these two species are part of the chain of reactions leading to the formation of OH and their discovery is another way to constrain the flux of cosmic rays in diffuse interstellar medium. The ratio OH^+ / H_2O^+ is between 5 and 6.5. As demonstrated by Neufeld et al. (2010), this can only be explained if the dissociation of OH^+ and H_2O^+ by electrons compete with reactions by H_2. Fig. 2 presents $N(OH^+)/N(H_2O^+)$ as a function of ζ obtained in PDR models for different densities. All models have an $A_V = 1$ and a UV radiation field equals to the ISRF. We can see that a ratio of 5 can be reached in models with low density and a high flux of cosmic rays (70×10^{-17} s^{-1}). This confirms Neufeld et al. (2010) results. Nevertheless, a more detailed models taking into account several low density clouds on the line of sight should be investigated.

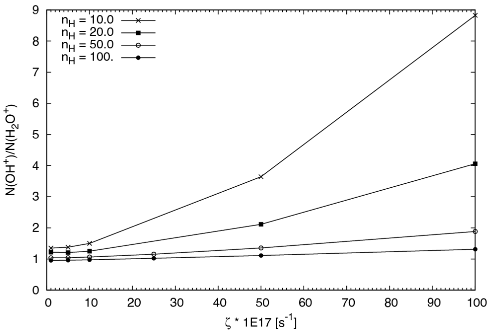

Fig. 2. Ratio $N(OH^+)$ / $N(H_2O^+)$ as a function of the flux of cosmic rays for different models with $A_V = 1$ illuminated by the interstellar standard radiation field.

6. Conclusions

The observation of OH, HD, H_3^+ and, with Herschel, OH^+ and H_2O^+ is a direct way to determine the flux of cosmic rays. McCall et al. (2003) showed that flux of cosmic ray in the diffuse interstellar medium is higher than what was thought previously. LePetit et al. (2004) showed that to deduce the flux of cosmic rays from molecules observations, one needs to use comprehensive models able to reproduce in a consistent way all the observations. They deduced that toward ζ Perseus, the flux of cosmic rays should be about 2.5×10^{-16} s^{-1}. Recent observations of H_3^+ in the CMZ and of OH^+ and H_2O^+ in the spiral arms are promising but, in these complex regions, observations of other species have to be done to interpret these observations properly.

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