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Cosmic ray dissociation of molecular hydrogen and dense cloud chemistry

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ABSTRACT

Dissociation of molecular hydrogen by secondary electrons produced by cosmic ray or X-ray ionization plays a crucial role in the chemistry of the densest part of molecular clouds. Here we study the effect of the mean kinetic energy of secondary electrons on this process. We compare predictions using a range of secondary electron energies and predictions of the cross sections with the values in the UMIST database. We find that the predicted column densities change by nearly one dex.

Keywords: ISM: molecules, ISM: abundances, ISM: cosmic rays, ISM: PDR

INTRODUCTION

Observationally, a significant fraction of atomic hydrogen (H) mixed with molecular hydrogen (H_2) is found to be present in the densest part of clouds that are shielded from the UV flux (Li & Goldsmith 2003). This is due to the dissociation of H_2 into atomic hydrogen by cosmic rays (CRs). The secondary electrons generated by CRs excite H_2 to its repulsive triplet state b that leads to dissociation of H_2 into two H atoms. The secondary electrons can also excite H_2 to the other triplet bound states e, a, and c, which will eventually decay down to the b state. In addition to this, CRs ionize H_2 into $H_2{}^+$. Padovani et al. (2018) showed that the ratio of dissociation rate to the ionization rate ($R_{diss/ion}$) varies between 0.6 to 0.7. The UMIST database (Millar et al. 1997) mentions 1.3×10^{-18} s^{-1} and 1.2×10^{-17} s^{-1} as the dissociation and ionization rates, respectively. This leads to $R_{diss/ion} = 0.1$ for UMIST rates. It is to be noted that the origin of the UMIST rates is not given. The abundance of H has important consequences for the chemical evolution of dense regions in the clouds, and this is affected by these rates.

Dalgarno et al. (1999) calculated the cross-sections for the H_2 dissociation as a function of the incident electron energy (their fig 4b). This cross-section is not uniform but rather decreases rapidly for higher energy. It is known that the secondary electrons have a broad range of energies. Spitzer & Tomasko (1968) states that the secondary electrons have kinetic energies between about 15 and 30 eV for inelastic collisions between 35 and 50 eV for elastic collisions. Dalgarno & Griffing (1958) and Glassgold & Langer (1973) report that the mean energy of the secondary electrons can be taken as 36 eV. Here we aim to study the effect of these different cross-sections at energies, 15 eV, 30 eV, and 36 eV on the cloud's chemistry and $R_{diss/ion}$ and compare this with the rate adopted by UMIST.

CALCULATIONS AND RESULTS

We consider a simple plane-parallel model with standard ISM abundances of gas and dust and set a constant kinetic temperature of 50 K. The hydrogen density is 10^5 cm^{-3}. Here we consider cosmic rays as the only source of radiation, and we block all UV flux and photoionization. The cosmic-ray ionization rate of H varies along different sight lines

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Table 1. Predicted column densities (cm^{-2}) in log scale

Species	15 eV	30 eV	36 eV	UMIST
H	18.73	18.32	18.09	17.28
H^+	12.09	11.90	11.82	11.92
OH	11.70	11.52	11.45	10.70
LiH	4.11	4.50	4.75	5.61
C_3H^+	12.54	12.71	12.77	12.61
C_2	17.09	17.23	17.28	16.47
C_3	16.29	16.46	16.52	16.36
CN	15.90	16.01	16.05	15.35
SiO	13.22	13.05	12.99	12.55
HS	13.85	13.67	13.61	13.54
NS	14.61	14.39	14.31	13.94
SO	11.25	10.86	10.72	10.92
$H_2{}^*$	13.96	13.54	13.31	12.51
$H_3{}^+$	13.86	13.85	13.84	12.68

(Indriolo et al. 2007). For our model, we consider this to be 10^{-16} s^{-1}. The cloud thickness is $A_V = 10$. All models presented here are calculated using version 17.01 of the spectral simulation code, CLOUDY (Ferland et al. 2013, 2017; Shaw et al. 2005).

We use figure 4b in Dalgarno et al. (1999) to evaluate the excitation cross section for the dissociative triplet state b (Shaw et al. 2008), rescale it in terms of the hydrogen ionization crosssection (Shemansky et al. 1985), and then multiply by the cosmic-ray excitation rate of Lyα at secondary electron energies at the three energies, 15 eV, 30eV, and 36 eV. For this simple model, the ratio $R_{diss/ion}$ is 9.93, 2.78, and 0.93 for cases with secondary electron energies at 15 eV, 30eV, and 36 eV, respectively.

Table 1 shows predicted column densities of the most-affected species and also shows the results using UMIST rates for the above mentioned two reactions, keeping other reactions the same. The UMIST rates predict the lowest H column density. Although the column densities in the lower levels of H_2 do not change very much, the column densities for higher levels ($H_2{}^*$) do change significantly. Note that the H_3^+ column density, the current gold standard for measuring the cosmic ray background (Indriolo et al. 2007), varies by one dex.

Earlier, Cloudy has used 20 eV secondary electrons as described in Shaw et al. (2008). In future versions of Cloudy, we will use 36 eV as the mean kinetic energy of the secondary electrons. The ideal calculation would solve for the cosmic ray secondary electron energy spectrum.

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