THE PHOTODISSOCIATION OF INTERSTELLAR CH^+

K. Kirby
Harvard-Smithsonian Center for Astrophysics

Abstract. Three new excited states of CH^+ which can be reached by a dipole transition from the ground state with photon energies less than 13.6 eV have been obtained from accurate theoretical calculations. As these states are unbound with respect to nuclear motion, photon absorption into them results in dissociation of the molecule. Photodissociation cross sections have been calculated, and the CH^+ photodissociation rates in the interstellar radiation field as a function of optical depth have been determined. The rates are approximately 500 times larger than previously assumed. We have compared these new photodissociation rates with the rates of other CH^+ destruction mechanisms in three different models of the interstellar medium. Photodissociation appears to be a significant destruction mechanism in any model requiring large interstellar radiation fields.

1. DESCRIPTION OF THEORETICAL CALCULATIONS

Using accurate configuration interaction methods Kirby, Saxon and Liu (1979a) have calculated energies and wavefunctions for seven previously undetermined states of CH^+ lying within $\sim$17 eV of the ground state. These excited states of $^1\Sigma^+$ and $^1\Pi$ symmetry which can be reached by a dipole transition from the ground $X^1\Sigma^+$ state are shown in Figure 1. The $X^1\Sigma^+$ and $A^1\Pi$ potential curves are known from previous theoretical work (Green et. al. 1972). The new states, labelled by numbers in Figure 1, are unbound with respect to nuclear motion, and electronic transitions to them will result in photodissociation of the CH^+. Dipole transition moments between the ground and excited electronic states have been computed as a function of internuclear separation (Kirby et al. 1979a) and used in the calculation of the photodissociation cross sections (Kirby et al. 1979b).

With photon energies $\leq$ 13.6 eV, dissociation from the ground vibrational state, v"=0 of the $X^1\Sigma^+$, takes place through the $2^1\Sigma^+$, $3^1\Sigma^+$ and $2^1\Pi$ states, producing $C(^1D)+H^+$ and $C(^1S)+H^+$ with maximum cross sections of $6x10^{-19}$ cm^2, $3x10^{-17}cm^2$ and $1.3x10^{-17}cm^2$, respectively.

B. H. Andrew (ed.), Interstellar Molecules, 283–286.

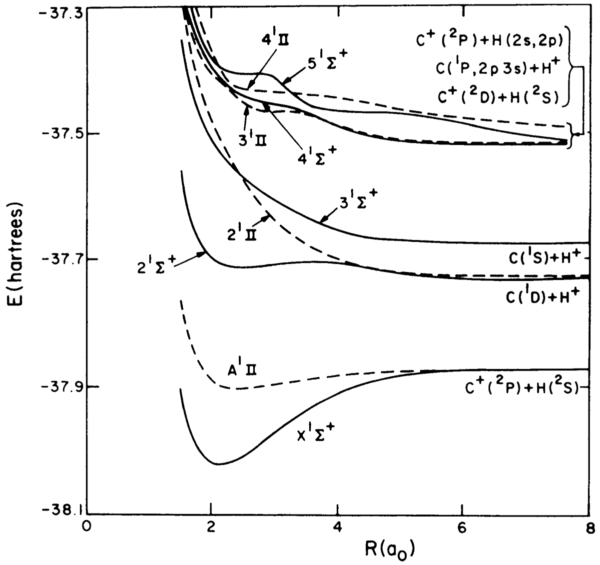

Figure 1. Potential curves of $^1\Sigma^+$ and $^1\Pi$ states of CH^+.

Previous estimates of the photodissociation rate of CH^+ were based on transitions from v"=0 to the $A^1\Pi$ state, producing $C^+(^2P)$+H. These new cross sections are more than two orders of magnitude larger than the X-A transition cross sections, and the possible ramifications for formation and destruction of CH^+ in the interstellar medium are examined in the next section.

2. PHOTODISSOCIATION RATES OF CH^+ IN INTERSTELLAR CLOUD MODELS

Photodissociation rates for transitions from v"=0 of the $X^1\Sigma^+$ state to the four CH^+ states lying below the Lyman limit have been calculated as a function of visual optical depth, τ_v, in an interstellar cloud (Kirby et.al. 1979b). The interstellar radiation field used was that of Draine (1978) for wavelengths less than 2300 Å, and that of Witt and Johnson (1973) for wavelengths greater than 2300 Å. At the surface of a cloud where τ_v=0, the overall photodissociation rate for CH^+ is $2\text{x}10^{-10}\ s^{-1}$.

In order to examine the effect of the large photodissociation rate on the CH^+ chemistry in diffuse interstellar clouds, we have compared the total rate for the photodissociation process:

$$CH^+ + h\nu \rightarrow C + H^+ \qquad k_1 = 2\text{x}10^{-10}s^{-1} \text{ for } \tau_v=0 \qquad (1)$$

with the rates of other destruction processes:

https://doi.org/10.1017/S0074180900072703 Published online by Cambridge University Press

Table 1. Parameters and Destruction Rates for CH^+ in the following models: S-W (Stecher and Williams 1974); B-D (Black and Dalgarno 1977); E-W (Elitzur and Watson 1978)

	Model Parameters					Destruction Rates			
	I	T °K	n(e)	n(H)	$n(H_2)$	Ik_1	$n(e)k_2$	$n(H_2)k_3$	$n(H)k_4$
S-W	1000*		3	100	100	$2x10^{-7}$	$1x10^{-7}$	$1x10^{-7}$	-*
B-D	2.5	110	0.06	300	100	$\sim 1x10^{-11}$	$1x10^{-8}$	$1x10^{-7}$	$8x10^{-10}$
		22	0.25	180	1160	$(\tau=1)$	$9x10^{-8}$	$1x10^{-6}$	$6x10^{-11}$
E-W	10*	4500	$6x10^{-3}$*	15	0.6	$2x10^{-9}$	$1x10^{-10}$	$6x10^{-10}$	$4x10^{-9}$

$$CH^+ + e \rightarrow C + H \qquad k_2 = 10^{-7}(300/T)^{1/2} cm^3 s^{-1} \qquad (2)$$

$$CH^+ + H_2 \rightarrow CH_2^+ + H \qquad k_3 = 1x10^{-9} cm^3 s^{-1} \qquad (3)$$

$$CH^+ + H \rightarrow C^+ + H_2 \qquad k_4 = 7.5 \times 10^{-15} T^{5/4} c-^3 s^{-1} \qquad (4)$$

The values for the rate constants k_2, k_3 and k_4 have been taken from Dalgarno (1976). These rates vary, depending on the electron density, the gas temperature, the molecular and atomic hydrogen densities, and the strength of the interstellar radiation field.

We have examined three model interstellar situations, two of which have been constructed specifically to explain the CH^+ formation and abundance. The first five rows of Table 1 list the parameters characterizing the models which have either been given explicitly by the authors, or which we have deduced (in the latter case, these quantities are starred). The parameter I is the scaling factor multiplying the average interstellar radiation field of Witt and Johnson (1973).

The model of Stecher and Williams (1974) elaborates on the ideas of Bates and Spitzer (1951) proposing evaporation of CH_4 from grain mantles, its subsequent photodissociation and ultimate photoionization of CH to give CH^+. Strong radiation fields generated by the close proximity of a hot star are needed to maintain an ionization rate for CH of $10^{-7} s^{-1}$. The two component model of Black and Dalgarno (1977) was constructed for the ζ Ophiuchi cloud and seriously underestimates the abundance of CH^+. In Table I the values applicable to the warm, diffuse outer zone always appear above those applicable to the cooler, denser inner zone. Elitzur and Watson (1978) propose formation of CH^+ through the endothermic reaction of $C^+ + H_2 \rightleftarrows CH^+ + H$ in the hot gas immediately behind shock fronts.

The destruction rates of CH^+ in s^{-1} are given in the second half of Table 1 for the various models. The photodissociation rates appear in the row labeled Ik_1, and the rates for reactions (2), (3), and (4) appear in successive rows. In the Black and Dalgarno (1979) model the primary destruction mechanism for CH^+ is reaction with molecular hydrogen, and photodissociation is comparatively insignificant. In the models of Stecher and Williams (1974) and of Elitzur and Watson (1978) which have enhanced radiation fields, however, the photodissociation rates are comparable to the rates of the other removal mechanisms. Recently de Jong (1979) has suggested that the shocks in which the CH^+ is formed are located at the edges of interstellar clouds (E-W parameters in Table 1 but I = 1). In that case the general interstellar radiation field applies so that photodissociation of CH^+ becomes about one order of magnitude less efficient than destruction by collisions with H atoms.

REFERENCES

Bates, D.R. and Spitzer, L.: 1951, Ap. J. 113, pp. 441-463.
Black, J.H. and Dalgarno, A.: 1979, Ap. J. Suppl. 34, pp. 405-423.
Dalgarno, A.: 1976, *Atomic Processes and Applications*, ed. Burke, P.G. and Moiseiwitsch, B.L. (North Holland: Amsterdam) pp. 109-132.
de Jong, T.: 1979, submitted to Astron. and Astrophys.
Draine, B.T.: 1978, Ap. J. Suppl. 36, pp. 595-619.
Elitzur, M. and Watson, W.D.: 1978, Ap. J. 222, pp. L141-L144.
Green, S., Bagus, P.S., Liu, B., McLean, A.D. and Yoshimine, M.: 1972, Phys. Rev. A 5, pp. 1614-1618.
Kirby, K., Saxon, R.P. and Liu, B.: 1979a, J. Chem. Phys. to be published.
Kirby, K., Saxon, R.P., and Liu, B.: 1979b, Ap. J. 231, pp. 637-641.
Stecher, T.P., and Williams, D.A.: 1974, M.N.R.A.S. 168, pp. 23P-26P.
Uzer, T. and Dalgarno, A.: 1978, Chem. Phys. 32, pp. 301-303.

DISCUSSION FOLLOWING KIRBY

Elitzur: Our model has an extinction of .5 which will further decrease the importance of the CH^+ photodissociation.

Kirby: Nowhere in your published model (Elitzur and Watson, 1978) is there any indication of an extinction of 0.5. However, such an extinction would certainly decrease the relative importance of CH^+ photodissociation as a destruction mechanism.

https://doi.org/10.1017/S0074180900072703 Published online by Cambridge University Press