EXCITED HYDROGEN CHEMISTRY IN PROTOSTELLAR OUTFLOWS

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ABSTRACT. Chemical models of protostellar and other outflows have been reassessed in the light of new chemical data. In particular, reactions involving excited hydrogen (2s,p) are shown to be important in hot, dense outflows. The H(n=2) + H $\rightarrow$ H_2 + hν reaction is much less of a contributor to the H_2 formation rate than the recently measured H(n=2) + H $\rightarrow$ H_2^+ + e^- reaction, providing conditions allow the 0.75eV endothermicity of this reaction to be overcome.

1. Chemistry

We report here for the first time the significance of the associative ionization reaction:

$$H + H(n = 2) \longrightarrow H_2^+ + e^-. \quad (1)$$

Cross-sections for this reaction have been measured by Urbain *et al.* (1991). Using these we calculate rate coefficients (in $cm^3\ s^{-1}$) of: 1.7×10^{-13} at 3000K, 1.1×10^{-12} at 5000K, and 6.0×10^{-12} at 10000K. A good fit to the rate coefficient at T $\gtrsim$ 2500 K is given by:

$$k = 3.5\times10^{-14} + 3.1\times10^{-11}e^{-16355/T}\ cm^3s^{-1} \quad (2)$$

The reaction is endothermic by 0.75eV and the cross-section shows a secondary barrier of $\simeq$2eV. H_2 formation then occurs as a result of charge exchange:

$$H_2^+ + H \longrightarrow H_2 + H^+ \quad (3)$$

We expect this path is particularly important in the chemistry of protostellar outflows. In all cases of astrophysical interest it is faster than the radiative association reaction proposed by Latter and Black (1991):

$$H + H(n = 2) \longrightarrow H_2 + h\nu \quad (4)$$

Furthermore, the negative-ion H_2 formation route is ineffective in outflows from cool as well as hot stars because of photo-detachment of H^- in the IR radiation field. In short,

P. D. Singh (ed.), Astrochemistry of Cosmic Phenomena, 387–388.

reaction (1) is a major contributor to the H_2 formation rate in both (i) high-temperature, strongly irradiated regions where the n=2 level is well populated, (ii) cooler (3000 - 5000 K), denser regions. In (ii), lower ionization and large departures from LTE (eg. at 3000K, $H(n=2)/H^+ > 2\times10^{-4}$) are necessary for reaction (1) to be more important than direct radiative recombination of H^+ with H.

2. Models

We have tested the importance of the excited hydrogen chemistry in four situations: T-Tauri winds, cool neutral outflows, BN winds and the ejecta of supernovae.

In the case of T-Tauri winds and cool neutral outflows we have adapted the models of Rawlings *et al.* 1988 and a model of Glassgold *et al.* 1989 to accommodate the new chemistry. In both cases the initial ionization was calculated by balancing recombination against collisional ionization. The results show that within a few stellar radii H_2 is significantly enhanced on including reaction (1). However, at later times the temperature and density drop whilst, in the case of the T-Tauri wind, the ionization level remains quite high. At this stage radiative recombination of H^+ with H becomes relatively more efficient (see also Latter and Black's discussion of H(n=2) chemistry in the early universe). Note these calculations do not include Lyα trapping and so set a *lower* limit to the efficiency of the H(n=2) chemistry.

The winds associated with BN-type objects are hot, dense and fairly well ionized – the most promising conditions for the excited hydrogen reactions. In our model $R_* = 4\times10^{11}$ cm, $\dot{M} = 1.0\times10^{-6}$ $M_\odot yr^{-1}$, $v_\infty = 150$ km s^{-1}, and the underlying radiation field is a Kurucz model atmosphere for T_{eff}=25000K, log(g)=4.0. We adopt a slowly accelerating velocity law and a temperature profile consistent with the wind models of Drew (1989). Self-shielding for H_2, CO and the carbon continuum have been included. To begin with, we use a two-level H^o atom + continuum: transfer in Lyα is accounted for using escape probabilities based on the Sobolev approximation, and the effect of Balmer continuum opacity is included. For the initial conditions we assume that H(n=1)/H(n=2) are in detailed balance and that photoionization of H(n=2) balances case B recombination. Preliminary calculations confirm H_2 formation via reaction (1) is *very* important in hot, partly ionized winds.

In the case of supernovae we have looked at both the "core" and the "mantle" of the ejecta. Despite the presence of a strong, very non-thermal high energy electron flux in the core region, NLTE models of the ejecta of SN1987a (eg. Schmutz *et al.* 1990) show the departure coefficients for H^o n=1,2 and 3 are less than 10. Hence, as the temperature is also low (2-3000 K), there is unlikely to be a significant enhancement to the chemistry in the core. In the "mantle" region, observations indicate that the n=2 level may be markedly overpopulated. However, even here, the importance of excited hydrogen chemistry in SN1987a appears to be marginal.

In some situations, the reaction: $H(n=3) + H \longrightarrow H_2^+ + e^-$ may also be significant. It is exothermic by 1.14eV but no cross-sections are yet available.

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