

# EQUILIBRIUM CONSTANTS OF THE MOLECULAR ION $\text{H}_3^+$

(Letter to the Editor)

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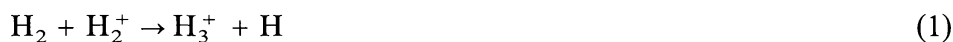
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**Abstract.** The  $\text{H}_3^+$  molecular ion plays an important role in the chemistry of astronomical objects as it protonates the neutral species. The authors have recently calculated the partition functions of  $\text{H}_3^+$  which may be used to compute the equilibrium constants for the chemical reaction  $\text{H}_2 + \text{H}_2^+ \rightarrow \text{H}_3^+ + \text{H}$ . In this short communication we have calculated the equilibrium constants for the temperature range from 500 to 8000 K. The results are also presented in the polynomial form.

## 1. Introduction

The importance of the molecular ion  $\text{H}_3^+$  has been discussed in our paper (Chandra *et al.*, 1991) where the partition functions of the ion were calculated. The detection of  $\text{H}_3^+$  in the planet Jupiter (Drossart *et al.*, 1989) has provided an impetus. After publishing the calculations for the partition functions, the authors realised that the equilibrium constants for the reaction



should be made available in the easy form. Therefore, in this short communication, the equilibrium constants for the reaction are calculated.

## 2. Equilibrium Constants

The equilibrium constants for the reaction (1) is defined in Herzberg (1945) as

$$K_p = \frac{Q_{\text{H}_3^+} Q_{\text{H}}}{Q_{\text{H}_2} Q_{\text{H}_2^+}} \exp(-\Delta E_0^0/RT), \quad (2)$$

where  $Q$ 's are the total partitions referred to the lowest energy level of the molecule (or atom). The total partition function is the product of translational and internal partition functions. Thus, Equation (2) can be simplified to

$$K_p = \left(\frac{3}{4}\right)^{1.5} \frac{Q_{\text{int H}_3^+} Q_{\text{int H}}}{Q_{\text{int H}_2} Q_{\text{int H}_2^+}} \exp(-\Delta E_0^0/RT), \quad (3)$$

where  $\Delta E_0^0$  is the total standard molar zero-point energy;  $T$ , the temperature; and  $R$ , the molar gas constant. Since  $\text{H}_3^+$  cannot exist in the level  $J = 0$ , the energy of the lowest possible level  $J = 1, K = 1$ , is  $64.117 \text{ cm}^{-1}$ . Therefore, the value of  $\Delta E_0^0$  was changed by  $64.117 \text{ cm}^{-1}$  and was taken to be  $\Delta E_0^0 = 1.703 \text{ eV} - 64.117 \text{ cm}^{-1} = 1.695 \text{ eV}$ . The required internal partition functions of  $\text{H}_2$ ,  $\text{H}_2^+$ , and  $\text{H}$  are reported by Sauval and Tatum (1984). The equilibrium constants for the reaction as a function of temperature are shown in Figure 1. The plot of  $\log K_p$  versus  $\log T$  is a smooth curve and can be fitted

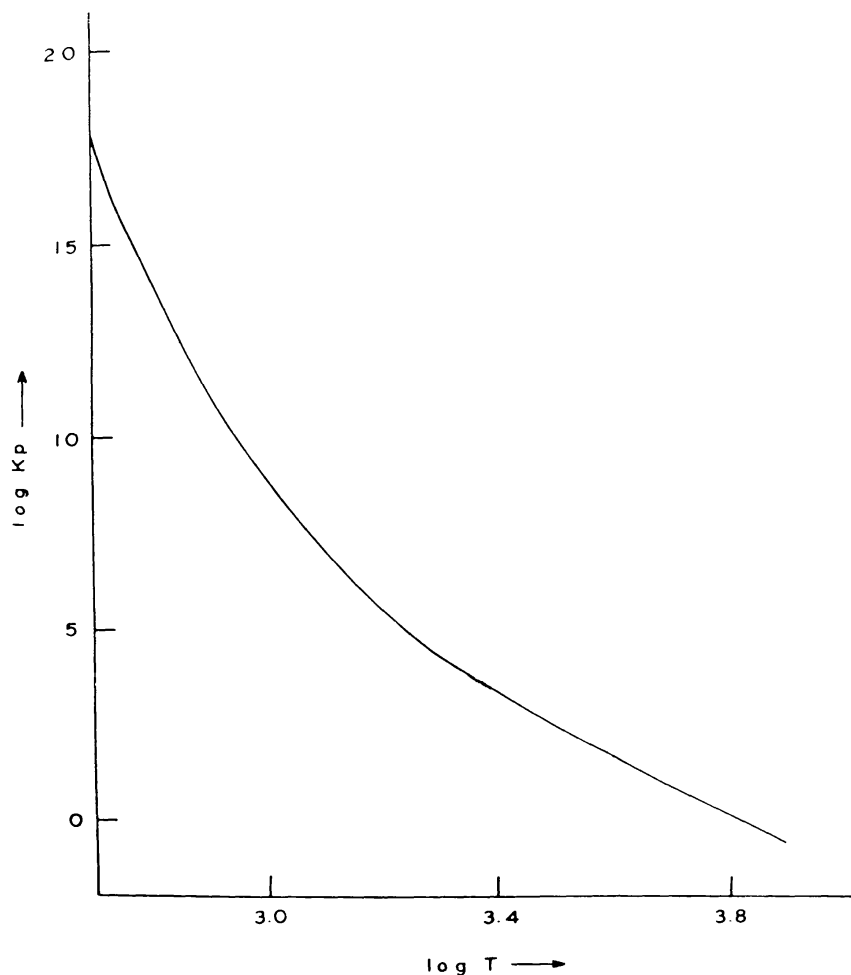


Fig. 1. The variation of the equilibrium constant  $K_p$  as a function of kinetic temperature  $T$ . The base of the logarithm is 10.

in the polynomial form

$$\log K_p = \sum_{n=0}^5 C_n ((\log T))^n, \quad (4)$$

where

$$C_0 = 2153.007947, \quad C_1 = -2653.346579,$$

$$\begin{aligned} C_2 &= 1327.184108, & C_3 &= -335.521017, \\ C_4 &= 42.793159, & C_5 &= -2.202111. \end{aligned}$$

### 3. Discussion

The equilibrium constants may be used to compute the LTE abundances of  $\text{H}_3^+$  in astronomical objects. In principle, the calculations are straightforward when the required partition functions are available. However, an astrophysicist may not have enough time to look into the details of the spectroscopic part of  $\text{H}_3^+$  and may not take a note that the lowest possible state of  $\text{H}_3^+$  is at  $64.117 \text{ cm}^{-1}$  and not at  $0 \text{ cm}^{-1}$ . Therefore, the purpose of this short communication is to present the equilibrium constants for the reaction in the easily accessible form.

### Acknowledgements

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