## What is H<sub>3</sub><sup>+</sup>?

Ben McCall

- $\rightarrow$  Equilateral triangle structure
- $\rightarrow$  Simplest stable polyatomic molecule
- $\rightarrow$  No stable excited electronic states
- $\rightarrow$  No allowed rotational spectrum
- $\rightarrow$  Laboratory spectrum obtained in 1980



# Formation of H<sub>3</sub><sup>+</sup><sub>Ben McCall</sub>

<u>Step 1</u>: Cosmic-ray ionization of H<sub>2</sub>:

 $H_2 \xrightarrow{\text{cosmic ray}} H_2^+ + e^-$ Rate =  $\zeta \cdot n(H_2)$ 

<u>Step 2</u>: Ion-Molecule reaction with H<sub>2</sub>:

$$H_2 + H_2^+ \rightarrow H_3^+ + H$$

[occurs on every collision]

The cosmic-ray ionization rate is estimated from various methods to be  $\zeta \sim 10^{-17} \text{ s}^{-1}$ . For a dense cloud with  $n(H_2) \sim 10^5 \text{ cm}^{-3}$ , the rate of formation of  $H_3^+$  is  $\sim 10^{-12} \text{ cm}^{-3} \text{ s}^{-1}$ .

#### Ion-Neutral Chemistry Ben McCall

$$H_{3}^{+} + CO \rightarrow HCO^{+} + H_{2}$$
$$H_{3}^{+} + X \rightarrow HX^{+} + H_{2}$$

 $HX^{+} + Y \rightarrow XY^{+} + H$ 

H<sub>3</sub><sup>+</sup> initiates a network of ion-molecule chemical reactions, leading to the production of H<sub>2</sub>O and other molecules. Were

Earth's oceans made by  $H_3^+$ ?

The destruction of  $H_3^+$  in molecular cloud is dominated by reaction with the most abundant reaction partner, CO. This rate can be expressed as  $k_{CO} n(H_3^+) n(CO)$ .

> $k_{CO} \sim 2 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ (measured in lab)



#### H<sub>3</sub><sup>+</sup> Number Density Ben McCall

Assuming steady-state, the  $H_3^+$  number density can be derived by equating the rates of formation and destruction.

Formation Rate (cosmic rays): $\zeta$  n(H2)Destruction Rate (rxn with CO): $k_{CO}$  n(CO) n(H3+)

Rearrange the equation  $\zeta n(H_2) = k_{CO} n(CO) n(H_3^+)$  to find:

$$n(H_3^+) = \frac{\zeta}{k_{CO}} \frac{n(H_2)}{n(CO)} = \text{constant!}$$

 $\begin{array}{ll} \underline{Adopted \ values:} \\ \zeta \sim 10^{-17} \ s^{-1} & (derived \ from \ observations) \\ k_{CO} = 2 \times 10^{-9} \ cm^3 \ s^{-1} & (measured \ in \ lab) \\ n(H_2)/n(CO) \sim 6.7 \times 10^3 & (from \ model \ calculations) \end{array}$ 

 $n(H_3^+)$  is constant ~  $3 \times 10^{-5}$  cm<sup>-3</sup> which is independent of the density of the cloud!

### H<sub>3</sub><sup>+</sup> Transitions

Ben McCall



#### Telescopes & Instruments Ben McCall



United Kingdom Infrared Telescope (UKIRT) Mauna Kea, Hawaii



Cooled Grating Spectrometer 4 (CGS4)  $R \sim 20,000$ 



Nicholas U. Mayall Telescope Kitt Peak, AZ



Phoenix Spectrometer R ~30,000



Molecular Cloud GL2136. This source provided the first detection of interstellar  $H_3^+$ . Using the CGS4 spectrometer at UKIRT, it observed at two times separated by nearly three months. The Earth's orbital motion around the Sun caused the spectral lines of  $H_3^+$  to be Doppler shifted – compelling evidence that the lines are genuine.

 $N_{para} = 4.0(9) \times 10^{14} \text{ cm}^{-2}$  $N_{ortho} = 3.0(6) \times 10^{14} \text{ cm}^{-2}$ 

> T. R. Geballe & T. Oka Nature 384, 334 (1996)

#### H<sub>3</sub><sup>+</sup> – Interstellar Probe Ben McCall

Measurements of  $H_3^+$  provide:

- $\rightarrow$  path length of cloud
- $\rightarrow$  number density of H<sub>2</sub>
- $\rightarrow$  kinetic temperature

Path Length:

$$L = \frac{N(H_3^+)}{n(H_3^+)} = \frac{3 \times 10^{14} \text{ cm}^{-2}}{3 \times 10^{-5} \text{ cm}^{-3}} = 10^{19} \text{ cm} \approx 3 \text{ pc}$$

Number Density:

$$n(H_2) = \frac{N(H_2)}{L} = \frac{10^{24} \text{ cm}^{-2}}{10^{19} \text{ cm}} = 10^5 \text{ cm}^{-3}$$

Temperature:

$$\frac{N_{ortho}(H_3^+)}{N_{para}(H_3^+)} = \frac{g_{ortho}}{g_{para}} e^{-\frac{\Delta E}{kT}} = 2e^{-\frac{32.87}{T}}$$

$$\Rightarrow$$
 T ~ 27 K

