# State-to-state astrochemistry in the primordial Universe

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## Context

Star formation :

- Stars form in molecular clouds through gravitational collapse.
- Internal energy of the cloud (pressure due to its temperature) opposes gravitational forces, hindering the collapse.
- Collapse proceeds thanks to the cooling of the cloud, a process that reduces its internal energy.
- Cooling proceeds mainly through line emission of some species (including CO, $H_2O$, etc.) and continuum emission of the dust.

Primordial Universe and first stars :

- In the primordial Universe, prior to first stars, there are only light elements : H, D, He (+ Li and B in traces).
- Very different chemistry : main species include $H_2$, HD, $H^-$, $H_2^+$, $HeH^+$.
- No dust, only gaseous species.
- Main coolants for the gas are $H_2$ and HD.

$\Rightarrow$ Influence on first stars formation ?

## Reaction rate coefficients

In a chemical network, the variation of the density $n_A$ of a species $A$ is given by :

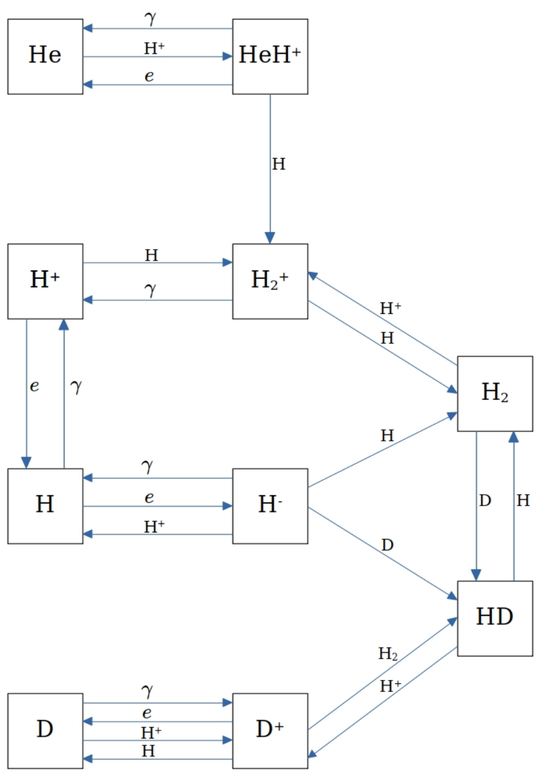
$$\frac{dn_A}{dt} = \sum_{prod} k_i(T) n_{r1} n_{r2} - \sum_{dest} k_j(T) n_A n_{r'}$$

where reactions $i$ of reactants $r1$ and $r2$ produce the species $A$ and reactions $j$ destroy the species $A$ and $r'$. $n$ denote the density of the different species and are in $cm^{-3}$. $k_i(T)$ is the reaction rate coefficient of reaction $i$ (in $cm^3.s^{-1}$) and depends only of the temperature.

## New chemical network

Based on the minimal network for primordial chemistry described by Galli & Palla [1], it concerns 11 species involved in 23 reactions.
Main changes are :

- Lithium chemistry removed because of very low abundance of lithium,
- 4 new reactions added (in red in the table of Figure 1).




| | reaction |
|---|---|
| H1 | $H^+ + e^- \rightarrow H + \gamma$ |
| H2 | $H + \gamma \rightarrow H^+ + e^-$ |
| H3 | $H^- + \gamma \rightarrow H + e^-$ |
| H4 | $H + e^- \rightarrow H^- + \gamma$ |
| H5 | $H^- + H \rightarrow H_2 + e^-$ |
| H6 | $H^- + H^+ \rightarrow H + H$ |
| H7 | $H + H^+ \rightarrow H_2^+ + \gamma$ |
| H8 | $H_2^+ + \gamma \rightarrow H + H^+$ |
| H9 | $H_2^+ + H \rightarrow H_2 + H^+$ |
| H10 | $H_2 + H^+ \rightarrow H_2^+ + H$ |
| D1 | $D^+ + e^- \rightarrow D + \gamma$ |
| D2 | $D + \gamma \rightarrow D^+ + e^-$ |
| D3 | $D + H^+ \rightarrow D^+ + H$ |
| D4 | $D^+ + H \rightarrow D + H^+$ |
| D5 | $D^+ + H_2 \rightarrow H^+ + HD$ |
| D6 | $HD + H^+ \rightarrow H_2 + D^+$ |
| D7 | $D + H_2 \rightarrow HD + H$ |
| D8 | $HD + H \rightarrow H_2 + D$ |
| D9 | $H^- + D \rightarrow HD + e^-$ |
| He1 | $He + H^+ \rightarrow HeH^+ + \gamma$ |
| He2 | $HeH^+ + H \rightarrow He + H_2^+$ |
| He3 | $HeH^+ + e^- \rightarrow He + H$ |
| He4 | $HeH^+ + \gamma \rightarrow He + H^+$ |

Figure 1 – Our present chemical network for primordial chemistry

The rate coefficients were updated based on recent available experimental results and/or theoretical calculations.
All our rate coefficients are fitted with modified Arrhenius form :

$$k(T) = a\,(T/300)^b \exp(-c/T)$$

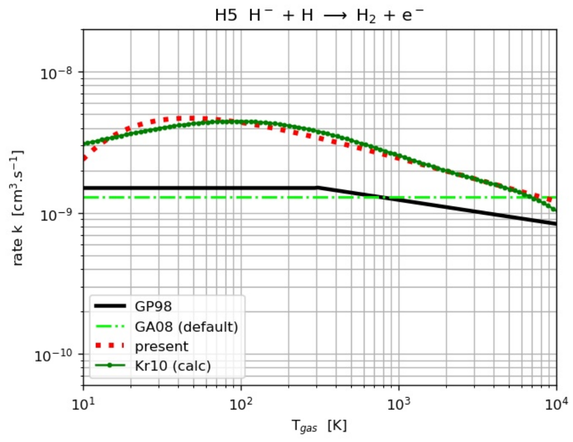



Figure 2 – Update of the rate coefficient of reaction H5 of our network. Previous rate are from Galli & Palla [1] and from Glover & Abel [2]. Present rate is a fit of the results of Kreckel et al. [3].

Our fits are valid between 10 K and 10,000 K and are accurate within a factor of 2-3.

## $H_2$ - H collisions

Collisional excitation of $H_2$ by H is important for the calculation of the cooling of the gas by $H_2$.
Previous data are from Lique (2015) [4] and needed to be recalculated at low temperature ($< 100$ K).

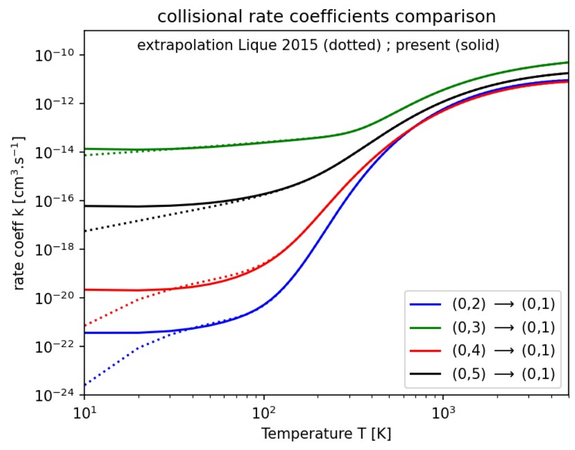



Figure 3 – Comparisons of the previous and the newly recalculated rate coefficients

We can see important changes in the rate coefficients at low temperature, by up to several orders of magnitude.
These results are also relevant for interstellar regions like PDRs as $H_2$ and H are among the most abundant elements in the Universe.

## Ongoing work and perspectives

- Computing state-of-the-art state-to-state reaction rates for the collisional excitation of $H_2$ by $H^+$ and He (main colliders with H) ;
- Modelling of primordial gas expansion and collapse using our upgraded chemical network to assess the roles and influence of the chemistry ;
- Introduction of state-to-state chemistry in our network.

## References

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