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Cosmological Implications of the Uncertainty in Astrochemical Rate Coefficients

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ABSTRACT

The cooling of neutral gas of primordial composition, or with very low levels of metal enrichment, depends crucially on the formation of molecular coolants, such as H_2 and HD within the gas. Although the chemical reactions involved in the formation and destruction of these molecules are well known, the same cannot be said for the rate coefficients of these reactions, some of which are uncertain by an order of magnitude. Here we discuss two reactions for which large uncertainties exist – the formation of H_2 by associative detachment of H^- with H and the destruction of H^- by mutual neutralization with protons. We show that these uncertainties can have a dramatic impact on the effectiveness of cooling during protogalactic collapse.

1. Primordial H_2 Chemistry

In the early universe, during the epoch of first star formation H_2 forms primarily via the radiative association process

$$\mathrm{H} + \mathrm{e}^- \rightarrow \mathrm{H}^- + \mathrm{h}\nu \tag{1}$$

followed by the associative detachment reaction

$$\mathrm{H}^- + \mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{e}^-. \tag{2}$$

For gas with a high fractional ionization, H^- is also destroyed rapidly by

$$\mathrm{H}^- + \mathrm{H}^+ \rightarrow \mathrm{H} + \mathrm{H} \tag{3}$$

However, the rate coefficients for reactions 2 and reaction 3 are both highly uncertain, as shown respectively in figure 1 below. Here we report on some of the cosmological implications of these uncertainties. A more detailed discussion is given in Glover et al. (2006).

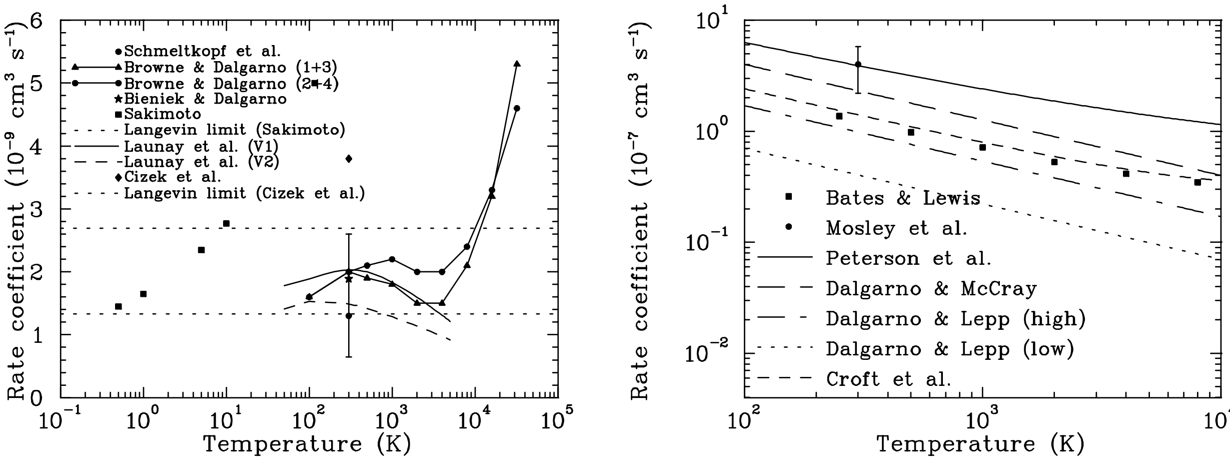

Fig. 1.— A summary of the various values found in the literature for the associative detachment rate coefficient for reaction 2 (left) and the mutual neutralization rate coefficient for reaction 3 (right). See Glover et al. (2006) for a fuller discussion.

2. Simulations

To study the impact of these astrochemical rate coefficient uncertainties, we have simulated the chemistry, cooling, and collapse of initially ionized gas into small protogalactic halos. Our simulations use a modified version of the GADGET smoothed particle hydrodynamics (SPH) code (Springer et al. 2001), to which we have added a treatment of primordial cooling and chemistry. For full details of the code see Glover et al. (2006). We simulate collapse at $z = 20$ into 10^7 $M_\odot$ dark matter halos, with various levels of background radiation. For each set of parameters, we perform 9 runs, with different combinations of values for the associative detachment and mutual neutralization rate coefficients. Between them, these combinations span the full range of plausible values.

We initialized each of our simulations at a redshift z = 20 and allowed them to run for 220 Myr; given our adopted cosmological parameters, this interval corresponds to approximately 1.25 Hubble times, with the simulations terminating at a redshift $z = 11.2$. Protogalaxies that fail to cool and collapse during this interval are unlikely to get the chance to do so thereafter, as the typical interval between major mergers of dark matter halos is of the order of a Hubble time (Lacey & Cole 1993).

3. Results

Simulations were carried out for a wide range of initial conditions. A full discussion and presentation of our results is given in Glover et al. (2006). Representative results are shown in figure 2 for the model predicted central H_2 fractional abundance of the primordial gas

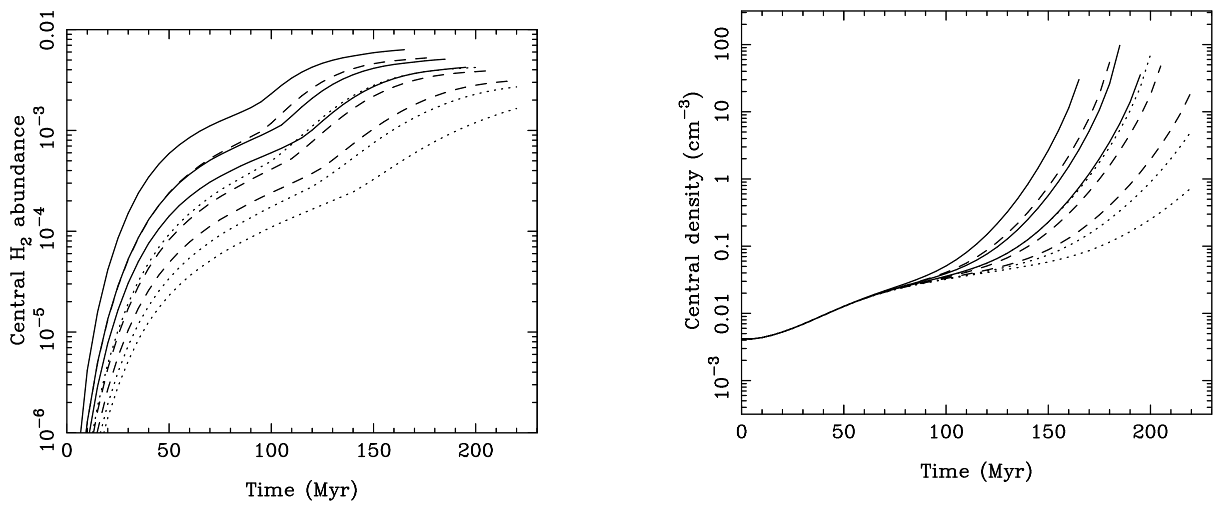

Fig. 2.— The evolution of the central H_2 abundance (left) and density (right) of a primordial gas cloud in a set of runs performed without an ultraviolet background. Mutual neutralization rates for these runs were taken from: Dalgarno & Lepp (1987) - solid lines; Croft et al. (1999) - dashed lines; and Peterson et al. (1971) - dotted lines. For each choice of mutual neutralization rate, three different associative detachment rates were used – the measured value of Schmeltekopf et al. (1967), which has a factor of at least two uncertainty, along with values 3.85 times larger and 2 times smaller to represent the range of published values for this reaction.

cloud and for the central density of the gas.

4. Summary

We have found that uncertainties in the associative detachment and mutual neutralization rate coefficients lead to uncertainties in the H_2 formation rate and the final H_2 fraction. These uncertainties have a measurable impact on the thermal and dynamical evolution of the collapsing gas. Though not shown here, the effect is particularly large when a UV field is present. In those cases, the final H_2 abundance may be uncertain by as much as a factor of 100. In summary, the predicted ability of the gas to cool in a given model protogalaxy depends in part on the choice of chemical rate coefficients used.

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