Formation of small molecules in interstellar space

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It is essential to know the roles of gas-phase and gas-grain processes for understanding the chemical evolution of the interstellar medium (ISM). In this work we investigate the formation of small molecules through radiative association. In radiative association two species collide and during the collision a photon is emitted, which carries away enough energy that the fragments become bound to each other. The emission of the photon is an improbable event giving small cross sections for molecule formation through radiative association. However, since the ISM is so dilute, energy loss by three-body collisions are even less likely. Thus radiative association can still be an important process for forming new molecules, particularly in dust poor regions.

Successful experimental measurements of radiative association rate constants for small molecules are few due to the small cross sections. It is thus of interest to perform theoretical calculations to estimate these rate constants. Here we perform quantum dynamical calculations of cross sections and rate constants for the formation of CO [1,2], HCO [3], $(NaH_2)^+$ [4] and $(AlH_2)^+$[5] through radiative association.

CO and HCO may be important species in the formation of complex organic molecules in space. It has for instance been proposed that a possible route for methanol formation could be to successively add H to CO [6]:

$CO \rightarrow HCO \rightarrow H_2CO \rightarrow H_3CO \rightarrow H_3COH$

The formation of CO by radiative association was calculated both for forming ^{12}CO and ^{13}CO. Surprisingly large isotope effects were obtained, which will be mentioned and discussed.

The thermal rate constants that we calculate for the H + CO radiative association are so small that in a cold interstellar medium this cannot be the process in the first step of the sequence shown above leading to the formation of methanol.

I will also bring up radiative association between H_2 (D_2) and Na^+ or Al^+ to form $(NaH_2)^+$ or $(AlH_2)^+$ and the deuterated versions. For $(AlH_2)^+$ formation we find the rate constant to be 3-4 orders of magnitude larger than the previous calculation by Petrie & Dunbar, but still too small to matter in astrochemistry. The $(NaH_2)^+$ formation on the other hand is fast enough that it should be included in chemistry models of dense molecular clouds.

References

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