Gas-phase formation of interstellar methyl cyanide: review and new theoretical calculations

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Recent studies suggest that nitrile-bearing molecules, characterised by the C≡N functionality, played a crucial role in prebiotic chemistry in the syntheses of RNA and protein precursors [1, 2, 3]. Methyl cyanide (CH_3CN) is one of the most abundant interstellar complex organic molecules and one of the widely detected, but its formation is still highly debated. Thus, we present a new chemical network (Figure 1), including also the isomer CH_3NC, in which the kinetic rates of the reactions have been reviewed and new paths have been included. Reactions 1) CH_4^+ + HCN, 2) $CH_3OH_2^+$ + HCN, 3) $CH_3OH_2^+$ + HNC, 4) CH_3CNH^+ + NH_3 and 5) CH_3NCH^+ + NH_3 were not studied via laboratory or theoretical works in the appropriate temperature and density conditions of the Interstellar Medium (ISM), therefore we carried out quantum chemical calculations followed by a theoretical kinetic analysis (using a semiempirical entrance potential and RRKM theory) to obtain accurate values of the rate constants at low temperatures (5-300 K). We coupled our computations with a chemical modelling analysis to check the relative importance of all the reactions in the network, depending on the physical conditions. We found that the reactions with protonated methanol (2 and 3) show an important steric effect which lead to a low rate coefficient ($k \sim 10^{-11}$ cm^3 s^{-1}) but they may be important in warm regions of the interstellar medium such as hot corinos. Path 1 is shown to be quite inefficient due to a low abundance of methanol in the ISM. Reactions 4 and 5 have a rate coefficient of 9×10^{-10} cm^3 s^{-1}, which is in line with other proton transfer reactions, but the electron recombination remains the most efficient way to form CH_3CN from protonated methyl cyanide.

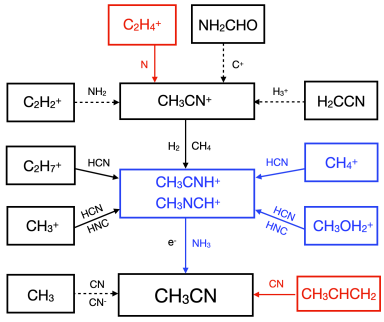

Figure 1 : Scheme of the gas-phase formation routes of CH_3CN. The blue boxes mark the reactions studied in the present work, while the red boxes mark the reactions which we suggest to remove from the network.

References

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