PHYS 192: Combined laboratory and theoretical studies on the formation of alcohols in the H_2O-rich ice phase of prestellar cores

Abstract:
The earliest stage in the star formation cycle at which solid-state complex organic molecules (COMs) can form is the dense cloud stage. As the density rises past ~10^3 H_2 molecules cm^{-3}, external UV photons are increasingly blocked from entering the cloud which also leads to a drop in the cloud temperature to 10-20 K. Under such conditions, COMs are likely formed through a non-energetic process, which is a radical-induced process that does not involve UV photons, electrons, and/or other energetic particles such as cosmic rays. This way of synthesizing COMs has been shown to be quite effective from recent solid-state laboratory experiments. Simple sugar-related species (e.g., glycolaldehyde), sugar alcohols (e.g., ethylene glycol and glycerol), aldehydes (e.g., propanal), and primary alcohols (e.g., n-propanol) have been formed from molecule and radical recombination in the CO + H reaction network a pathway that is observationally constrained to occur during the CO freeze-out stage of dense clouds. In this contribution, we show that COMs, and particularly alcohols, can already be formed before a majority of the CO freezes-out in the early period of the H_2O-rich ice phase. By utilizing an ultrahigh vacuum apparatus in combination with computational investigations, we show that the isomers, n- and i-propanol ($H_3CCH_2CH_2OH$ and $H_3CCHOHCH_3$) and n- and i-propenol ($H_3CCH=CHOH$ and $H_3CCOH=CH_2$), can be formed in the non-energetic reaction of propyne (H_3CCCH) + OH at 10 K. Gas-phase H_3CCCH has already been identified towards cold, dark and dense clouds, where it is expected to have an abundance < 1% relative to H_2O ice. The resulting 1:1 average abundance ratio of n-propanol:i-propanol found in the experiments is in agreement with the computationally-derived activation barriers and the finding that the geometric orientation between H_3CCCH and OH strongly influences the branching ratio. It is additionally shown that propene and propane ($H_3CCH=CH_2$ and $H_3CCH_2CH_3$) are formed from the hydrogenation of H_3CCCH, with a H_3CCCH: $H_3CCH=CH_2$: $H_3CCH_2CH_3$ abundance ratio of 9:1:2, respectively. The alcohols analyzed in this study are expected to be partially formed at the interface of the H_2O-rich ice and dust grain in dense clouds allowing preservation of alcohols and their extended counterparts containing H_3C-(CC)n-H structures (e.g., fatty alcohols) upon delivery to the early Earth.

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