A theoretical study of formation routes and dimerization of methanimine: implications for the aerosols presence in the upper atmosphere of Titan

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Methanimine is an important molecule in prebiotic chemistry since it is considered a possible precursor of the simplest amino acid, glycine, via its reactions with HCN (and then H_2O) or with formic acid (HCOOH). According to this suggestion, the simplest amino acid can be formed 'abiotically' starting from simple molecules relatively abundant in extraterrestrial environments and primitive Earth. Interestingly, methanimine has been observed in the upper atmosphere of Titan, which is believed to be somewhat reminiscent of the primeval atmosphere of Earth. Methanimine can be produced in the atmosphere of Titan by the reactions of N (^{2}D) with both methane and ethane, or by other simple processes, including the reaction between NH and CH_3 or reactions involving ionic species [1]. Recent models derived a larger quantity of methanimine than that inferred by the analysis of the ion spectra recorded by Cassini Ion Neutral Mass Spectrometer. Growing evidence suggests that nitrogen chemistry contributes to the formation of the haze aerosols in the Titan upper atmosphere. In this respect, since imines are well-known for their capability of polymerizing, CH_2NH is an excellent candidate to account for the nitrogen-rich aerosols of Titan through polymerization and copolymerization with other unsaturated nitriles or unsaturated hydrocarbons. Polymerization of methanimine provides an important contribution to the formation of the nitrogen-rich aerosols, but a quantitative inclusion of this process in the model could not be obtained as there is no information (either experimental or theoretical) on methanimine polymerization. Since the first step of polymerization is dimerization, in this contribution we report on a theoretical characterization of methanimine dimerization. Electronic structure calculations of the potential energy surfaces representing the reactions of electronically excited atomic nitrogen, N(^{2}D), with methane and ethane are also presented, as they are possible formation routes of methanimine under the conditions of the upper atmosphere of Titan.

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