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The N + CH3, N + H2CN and N + CH2 reactions: kinetics and products.

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The N(4S) + CH3 reaction is an important reaction for Titan's atmosphere as well as in evolved dense molecular clouds and in protoplanetary disks, leading to HCN through various reactions involving H2CN and CH2 radicals. We have studied the kinetics of the N + CH3 reaction between 147 K and 440 K using a fast flow reactor (300 K –440 K) and the CRESU technique (147 K). The reactants and various products (CH3, H2CN, CH2 radicals and H atoms) were detected either through mass spectroscopy after ionization at 10.54 eV or by VUV-LIF, the photons being produced through tripling in rare gas. By modelling the kinetics of CH3, H2CN and CH2 radicals for various conditions, we were able to determine the rate constant and the branching ratio of the N + H2CN reaction showing that the main products were CH2 + N2. We have performed DFT and ab-initio calculations on the N + H2CN reaction to elucidate the mechanisms involved. We have also measured the absolute ionization cross section of H2CN at 10.54 eV (using CH3 as reference) through the N + C2H5 reaction which lead to the same amount of CH3 and H2CN radicals.

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