EPSC Abstracts
Vol. 15, EPSC2021-268, 2021
https://doi.org/10.5194/epsc2021-268
Europlanet Science Congress 2021

Reactivity of N(^{2}D) atoms and of the cyano radical (CN) with vinyl cyanide (H_2CCHCN) in Titan's atmosphere: a combined crossed beam and theoretical study

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Several studies have reported model vertical profiles and/or abundance measurements for the main nitrile species observed in Titan's atmosphere including: hydrogen cyanide (HCN), cyanoacetylene (HC_3N), and vinyl cyanide (H_2CCHCN) [1-4]. One of the main mechanisms leading to the formation of these nitriles (molecules bearing the CN group) is the reaction of CN radicals with hydrocarbons (molecules with general formula C_xH_y) involving H elimination (*e.g.* CN + C_2H_4 = H_2CCHCN + H) or H abstraction (*e.g.* CN + CH_4 = HCN + CH_3) [5-9]. In this regard, it is worthwhile to highlight the recent spectroscopic detection of H_2CCHCN, obtained using archival data from the Atacama Large Millimeter/submillimeter Array (ALMA), because this species is the best candidate molecule to form stable cell membranes/vesicle structures of potential astrobiological importance in Titan's hydrocarbon-rich lakes and seas [10-12].

In the upper atmosphere of Saturn's moon, photolysis of N_2 and HCN leads to a continuous supply of reactive neutral species including N(^{4}S, ^{2}D) atoms and CN radicals [2, 13-16] that can further react with hydrocarbons and nitriles leading to two possible outcomes: 1) these reactions can directly contribute to the growth of molecular complexity, leading to a variety of N-rich organic species which, in turn, can act as (some of the) building blocks of life as we know it; 2) break the molecules into smaller but more stable fragments.

A detailed knowledge of the relevant potential energy surface for each reactive systems on the basis of quantum-mechanical calculations and laboratory experiments is of pivotal importance in identifying the nature of the primary products and estimating their branching ratios, and hence providing the modellers with solid ground to describe and predict the rich, complex chemical evolution of Titan's planetary atmosphere.

Within this framework, we will report on two elementary chemical processes: 1) N(^{2}D) + H_2CCHCN and 2) CN($X^2\Sigma^+$) + H_2CCHCN with emphasis on the N addition or CN addition (followed by H elimination) reactive channel by means of the crossed molecular beams (CMB) technique coupled with mass spectrometric detection and time-of-flight analysis, and we will report on the primary products from the analysis of our measurements. Additional insight on the micromechanism at play and the interpretation of the scattering results is given by new electronic structure calculations of stationary points and product energetics in the potential energy surface of the investigated systems. RRKM statistical calculations for the $CN(X^2\Sigma^+)$ + H_2CCHCN system allows us to derive the product branching ratios and rate constants under the conditions of the present experiments and of the atmosphere of Titan. Preliminary results and astrophysical implications will be presented.

ACKNOWLEDGMENTS:

This research was supported by the Italian Space Agency (ASI, DC-VUM-2017-034, Grant n° 2019-3 U.O Life in Space) and the Marie Skłodowska-Curie project "Astro-Chemical Origins" (ACO), grant agreement No 811312.

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