Simulating the Density of (Iso-)Nitrile Species in the Titan Atmosphere with a Coupled Ion-Neutral Photochemical Model

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Résumé

Recent observations from the Cassini spacecraft, the Herschel space observatory and the ALMA interferometer of radio telescopes drastically increased our knowledge of Titan's chemical composition. The combination of data retrieved by Cassini INMS, UVIS, and CIRS allows deriving the vertical profiles of half a dozen species from 1000 to 100 km, the HIFI instrument on Herschel reported on the first identification of HNC and ALMA observed multiple emission lines of C2H5CN. Partial data or upper limits are available for almost 20 other CHON neutral species. The INMS and CAPS instruments onboard Cassini also revealed the existence of numerous positive and negative ions in Titan's upper atmosphere.

We present the results of a 1D coupled ion-neutral photochemical model intended for the interpretation of the distribution of gaseous species in the Titan atmosphere. The model extends from the surface to the exobase. The atmospheric background, boundary conditions, vertical transport and aerosol opacity are all constrained by the Cassini-Huygens observations. The chemical network includes reactions between hydrocarbons, nitrogen and oxygen bearing species (including some species containing both nitrogen and oxygen, such as NO). It takes into account neutrals and both positive and negative ions with m/z extending up to about 100 u. Ab initio Transition State Theory calculations are performed in order to evaluate the rate coefficients and products for critical reactions.

We discuss the chemical and physical processes responsible for the production and loss of the (iso-)nitrile species detected on Titan. We find that these species are usually formed through a combination of ion and neutral reactions in the upper atmosphere and that ion chemistry is an efficient sink through proton transfer reactions and electron recombination. The calculated vertical profiles of HCN, HNC, CH3CN and HC3N generally agree with the existing observational constrains (from both neutrals and ions) although some small differences exist. However, the model predictions for C2H5CN in the stratosphere are about two

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orders of magnitude higher than the observations. This discrepancy is attributed to our poor knowledge of the chemistry of this species rather than to its sticking onto the aerosols.