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# Hydrogen isocyanide, HNC, in Titan's ionosphere

**V. Vuitton** (1), R. V. Yelle (2), S. J. Klippenstein (3), P. Lavvas (4), S. M. Hörst (5) and A. Bazin (1)
(1) IPAG, UMR CNRS 5274, Université Joseph Fourier Grenoble 1, France, (2) LPL, University of Arizona, Tucson AZ, USA, (3) Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL, USA, (4) GSMA, UMR CNRS 6089, Université de Reims Champagne-Ardenne, France, (5) CIRES, University of Colorado, Boulder CO, USA (veronique.vuitton@obs.ujf-grenoble.fr)

## Abstract

The first identification of hydrogen isocyanide, HNC, in Titan's atmosphere has recently been reported. Using a coupled ion-neutral photochemical model, we find that both neutral and ion chemistry contribute to the production and loss of HNC. According to our calculations, the HNC density reaches a peak of $\sim 10^6$ $cm^{-3}$ at an altitude of 950-1000 km. This translates into a a column density of $1.8 \times 10^{13}$ $cm^{-2}$ above 800 km, in fair agreement with the observations.

## 1. Introduction

Although hydrogen cyanide, HCN, has been detected on Titan as early as 1980 during the Voyager 1 encounter with this satellite, it took three more decades for HNC to be identified in this same atmosphere [5]. Observations using the HIFI instrument on the Herschel Space Observatory indicate that the bulk HNC is located above 400 km, with a column density in the range $(0.6 - 1.5) \times 10^{13}$ $cm^{-2}$, but the observations cannot establish its vertical profile.

Titan ionospheric models predict that $HCNH^+$ is one of the most abundant ions with a peak density on the order of 1000 $cm^{-3}$ around 1000-1200 km [3, 10]. After high-level ab initio quantum chemical investigations concurred that HNC is a major product of the dissociative recombination of $HCNH^+$ [9], it was soon recognized that HNC could have a significant density in Titan's upper thermosphere [7]. Simple calculations assuming formation through electron recombination of $HCNH^+$, loss through proton exchange reactions, and using known atmospheric properties, lead to and HNC column density of $7.0\times10^{11} - 5.2\times10^{12}$ $cm^{-2}$, which is somewhat marginally consistent with the measurements [5].

The production of HNC via neutral reactions has been investigated as well [1]. In this model, HNC is mostly produced from $H_2CN$ + H $\rightarrow$ HNC + H and to a lesser extent from $N(^4S)$ + $CH_2$ $\rightarrow$ HNC + H. It is mainly destroyed by its reaction with $N(^2D)$ above 1000 km and H at lower altitude. The column density obtained is $3.4 \times 10^{13}$ $cm^{-2}$, which is about 3 times higher than the value derived from the observations. It is argued that this discrepancy can be explained by the poor knowledge of three key reactions: H + HNC $\rightarrow$ H + HCN, H + $H_2CN$ $\rightarrow$ HNC/HCN + $H_2$ and $N(^2D)$ + HNC $\rightarrow$ $CN_2$ + H / CH + $N_2$.

## 2. Photochemical model

The 1-dimensional photochemical model of Titan used in this investigation is adapted from several elements described previously. The background atmosphere, eddy diffusion coefficient and electron temperature are based on Cassini observations [13, 6]. Detailed calculations for the energy deposition of photons and photoelectrons have been performed [4]. The chemical network includes hydrocarbons [11], nitrogen [14] and oxygen [2] bearing species and takes into account both neutral and ion chemistry [10].

We incorporate in this model 9 reactions leading to HNC production, 4 through neutral chemistry and 5 through dissociative recombination of nitrogen-bearing ions with electrons. All these reactions have been studied theoretically/ experimentally and are known to produce HNC. We also include 10 loss reactions with the most abundant neutral and ions present in the thermosphere. For the three reactions identified previously [1] as being responsible for HNC abundance uncertainties, we performed Ab Initio TST calculations in order to better predict their rate coefficient. For the other reactions the rate coefficients come for quantum chemical calculations when available [8] and otherwise have been assumed to be equal to the same rate coefficient as for HCN. For ion-neutral reactions we use capture rate coefficients obtained with the Su-Chesnavich expression [12].

## 3. Results and discussion

According to the calculations described above, the main HNC production reaction is H + $H_2CN$ with a column integrated rate of $5\times10^7$ $cm^{-2}$ $s^{-1}$, in good agreement with the previous model [1]. Recombination reactions ($HCNH^+$ + $e^-$ and to a lesser extent $C_2H_3CNH^+$ $e^-$) also contribute significantly with a total column integrated rate of $4\times10^7$ $cm^{-2}$ $s^{-1}$. $HCNH^+$ + $e^-$ is actually the main production reaction above 1150 km. The main losses are reaction with H below 1000 km and $C_2H_5^+$ above, with column integrated rates of 5 and $3\times10^7$ $cm^{-2}$ $s^{-1}$, respectively.

With the above production and loss rates, the bulk of the HNC is located above 800 km, with a density profile reaching a peak of $\sim 10^6$ $cm^{-3}$ at an altitude of 950-1000 km. This translates into a constant mixing ratio of $\sim 10^{-4}$ above 1050-1100 km and a column density of $1.8 \times 10^{13}$ $cm^{-2}$ above 800 km. This value is a factor of 2 higher than the column density retrieved from the observations assuming a constant mixing ratio profile above 800 km.

## 4. Conclusion

Following the previous calculations focusing on the formation of HNC in Titan's atmosphere [7, 1], we show that neutral chemistry and dissociative electron attachment of nitrogen-bearing ions contribute almost equally to the production of HNC. The calculated HNC column density is in fair agreement with the value retrieved from Herschel [5], but the vertical profile remains to be tested against the observations.


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