The Origins of Complex Organics in Cometary Comae

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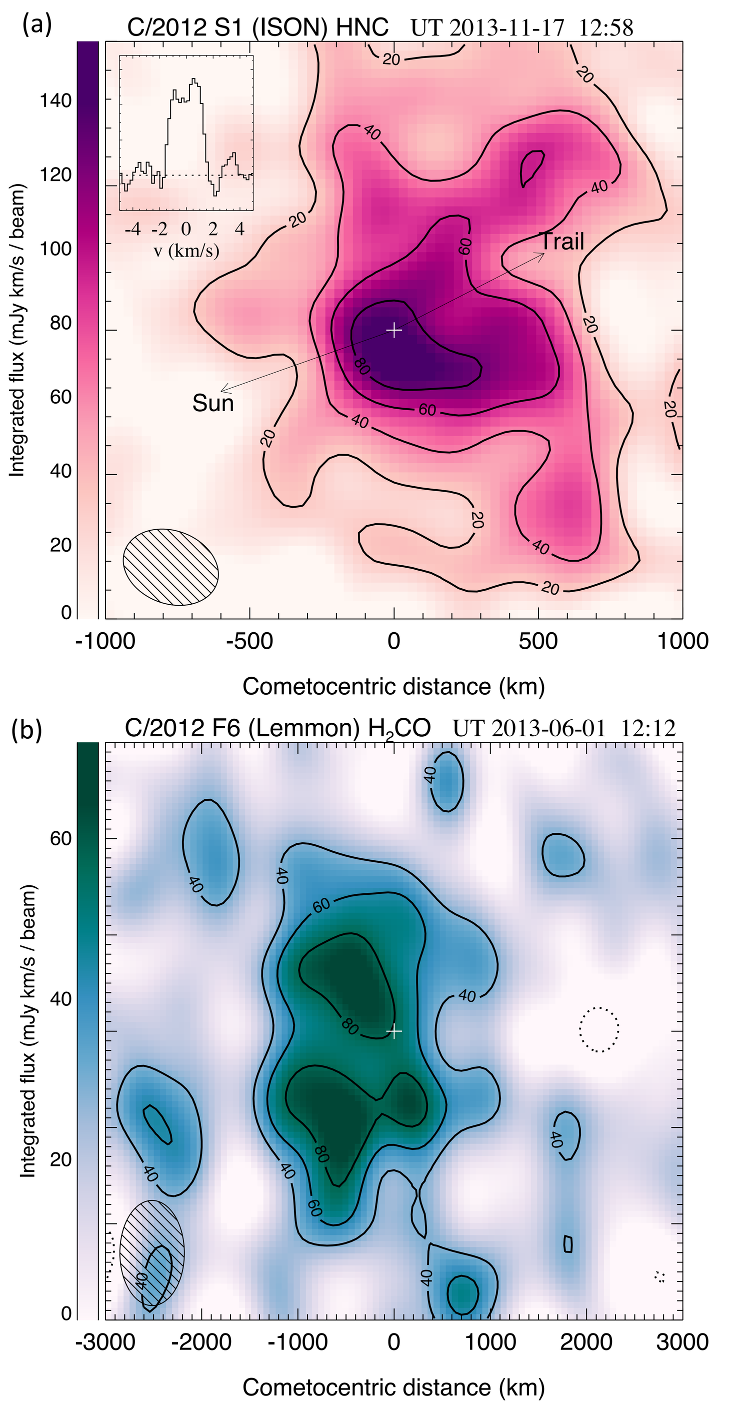
Introduction

Cometary ices have remained largely unprocessed since they accreted, so their study provides unique information on the earliest history of our Solar System, as well as providing insight into the chemical regents available for delivery to primitive planetary surfaces.

Cometary ice abundances are derived primarily through remote observations of their atmospheres (comae). However, through observations of spatially extended distributions (Fig. 1a,b), several commonly observed species (such as CN, C_2, HNC and H_2CO) are known to be produced as a result of coma photochemistry/thermal breakdown of dust, and may not be native to the nucleus. The assumption that complex organic molecules (such as HC_3N, NH_2CHO, and CH_3OCHO), commonly observed using single-dish radio spectroscopy are present in cometary ice is largely unproven. In fact, our new chemical/hydrodynamic coma model shows that some of these organics could instead be produced in the coma via gas-phase chemistry.

Here we present chemical model calculations for HC_3N and NH_2CHO, which reveal a coma origin for these species.



Fig, 1: ALMA maps of HNC and H_2CO in comets S1/ISON and F6/Lemmon, respectively, revealing clear extended production in the coma.

Chemical Model

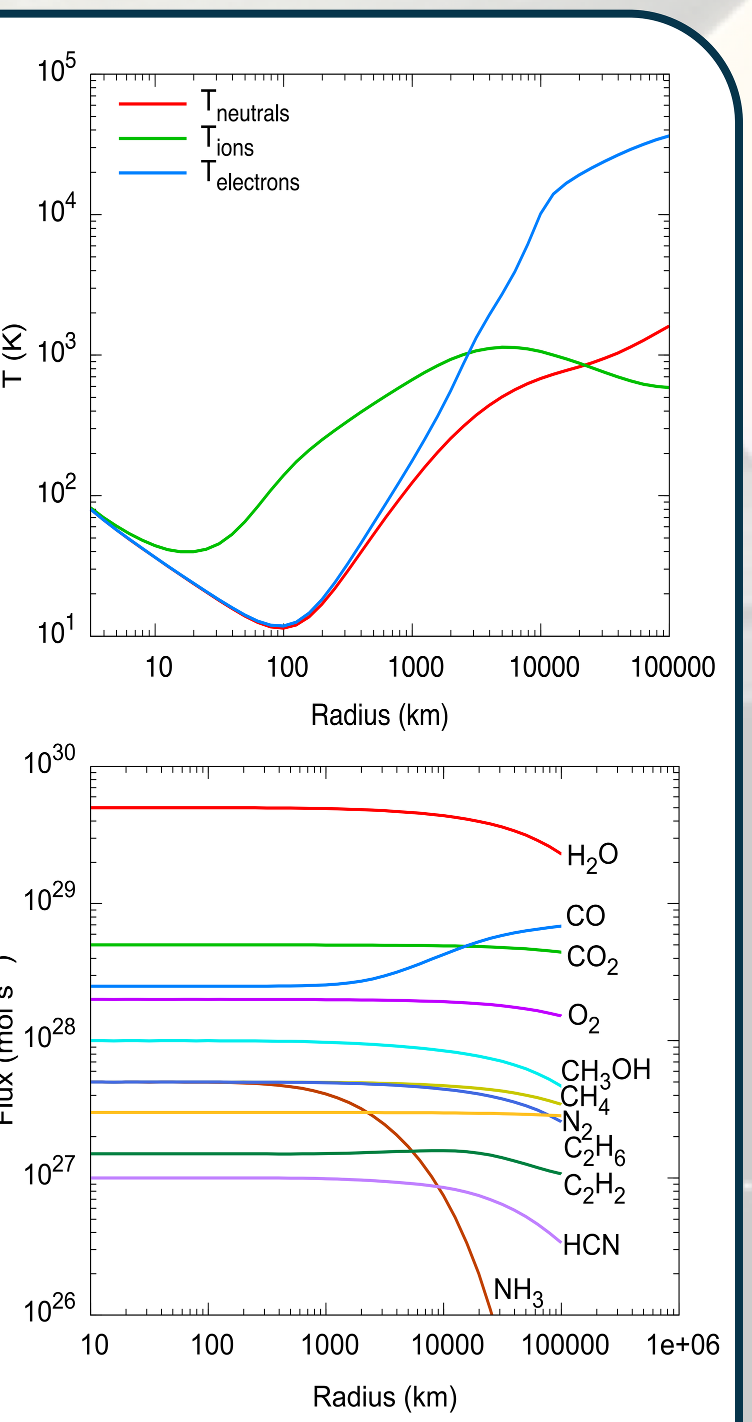
Our numerical model is based on the chemical/hydrodynamic coma code by Rodgers & Charnley (2002), with updated C,N,O chemistry from Cordiner & Charnley (2014). The coma abundances (n_i) of 280 species, and the temperatures (T_x) of the ion, neutral and electron fluids are calculated as a function distance (*R)* from the nucleus, using the DVODE package to solve the following coupled differential equations:

$$\frac{dn_i}{dR} = \frac{N_i}{v} - \frac{n_i}{v}\frac{dv}{dR} - \frac{2n_i}{R}$$

$$\frac{dT_x}{dR} = \frac{(\gamma_x - 1)T_x}{v}\left[\frac{G_x}{n_x k_B T_x} - \frac{2v}{R} - \frac{dv}{dR} - \frac{N_x}{(\gamma_x - 1)n_x}\right]$$

Where N_i are the source terms for the individual species (the sum over all chemical production and loss rates for species *i*), v is the coma outflow velocity, T_x, N_x are the respective temperature and source terms for fluid x, γ_x is the ratio of specific heats and G_x is the energy source term, defined as the sum of energetic contributions due to chemical reactions, collisions between ions, neutrals and electrons, and radiative energy loss from H_2O.

Coma gases (parent species) are released from the nucleus and follow a spherically symmetric expansion, whereupon they undergo photolysis by Solar radiation. The subsequent chemistry is modeled using 3851 reactions (involving 101 neutrals, 154 cations and 23 anions) from the latest version of the UMIST database for astrochemistry (McElroy et al. 2013). Solar photoreaction rates at 1 AU were taken from Huebner et al. (1992), Crovisier et al. (1994), Millar et al. (2007) and van Hemert & van Dishoeck (2008). Parent abundances are typical observed values from Mumma & Charnley (2011), and we assume an initial H_2O production rate of 5×10^{29} s^{-1}, which is typical for moderately bright cometary apparitions. We include H_2CO production in the coma through degradation of a macromolecular precursor, with a scale length of 1000 km.

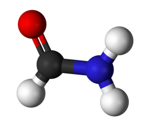


Fig, 2: Output from our chemical/hydrodynamic coma model showing (a) temperatures of the 3 fluids and (b) fluxes of parent molecules flowing out from the nucleus.

Table 1: Parent molecule abundances

Species	Abund. (%)	Species	Abund. (%)
H_2O	100	CH_4	1
CO_2	10	NH_3	1
CO	5	N_2	0.6
O_2	4	C_2H_2	0.3
CH_3OH	2	HCN	0.2
C_2H_6	1		

Results



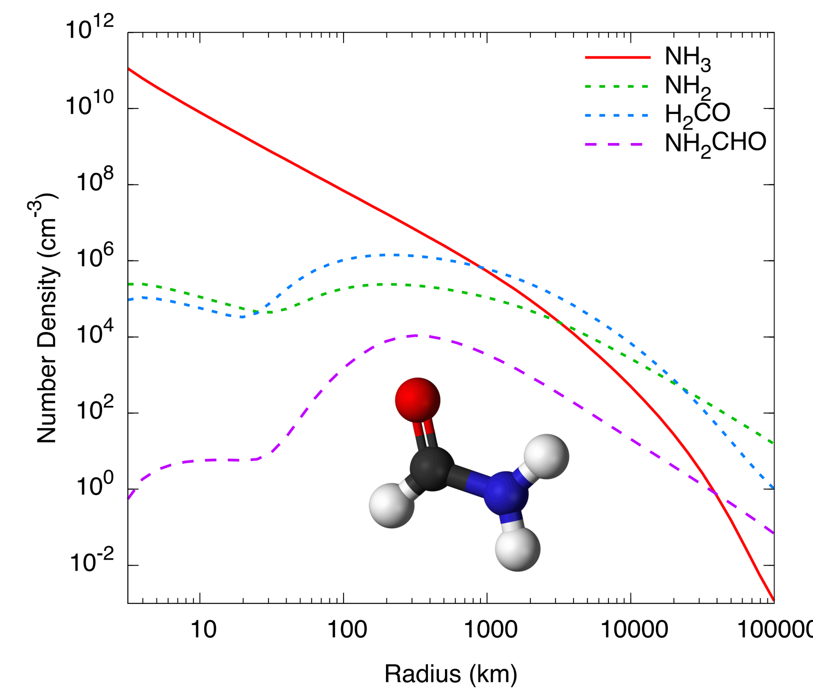
NH_2CHO

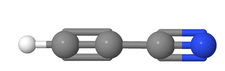
Barone et al. (2015) determined that NH_2CHO is produced rapidly at low temperatures by the reaction:

$NH_2 + H_2CO \rightarrow NH_2CHO + H$

Given the large abundances of NH_2 and H_2CO in our model coma, a substantial amount of NH_2CHO is thus synthesized (right), reaching a peak density a few hundred km from the nucleus.

The calculated NH_2CHO column density N = 5×10^{11} cm^{-2} is consistent with production rates observed using the IRAM 30-m radio telescope (Bockelee-Morvan & Biver 2017).





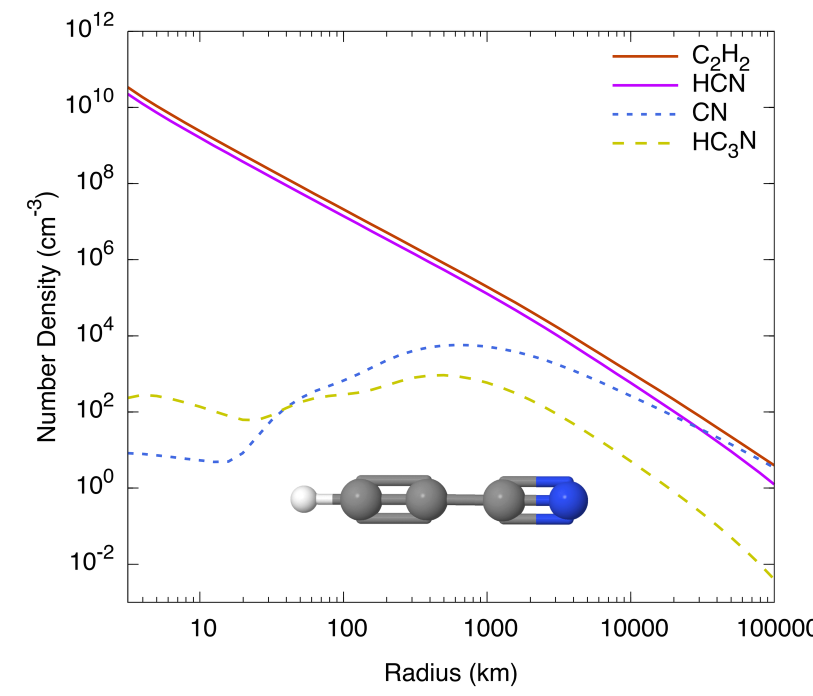
HC_3N

Laboratory experiments show that HC_3N is produced rapidly as follows (Sims et al. 1993):

$CN + C_2H_2 \rightarrow HC_3N + H$

The coma contains abundant CN and C_2H_2, so HC_3N is rapidly synthesized (right), with a peak density around 500 km from the nucleus.

The calculated HC_3N column density is N = 1×10^{11} cm^{-2}, which is consistent with the lower end of the range of observed production rates for this species.



Conclusion

- Our model shows that both NH_2CHO and HC_3N can be produced in cometary comae through gas-phase reactions involving simple chemical precursors known to be abundant in comets.
- Formamide (NH_2CHO) has been considered as a possible starting point for Earth's prebiotic synthesis (Saladino et al. 2012), so determining its abundance in cometary ice is of particular interest for astrobiology. Similarly, HC_3N has been implicated in the synthesis of nucleobases and amino acids (Ferris et al. 1968; Patel et al. 2015). These molecules are commonly detected in cometary comae, but have never before been mapped.
- We find that coma chemistry is a valid mechanism for the synthesis of complex organic molecules observed in comets at radio wavelengths, challenging the commonly-held assumption that these gases must originate from ices in the nucleus.
- The proposed coma synthesis of HC_3N and NH_2CHO can be tested through interferometric mapping using the Atacama Large Millimeter/submillimeter Array (ALMA), which will reveal, for the first time, their detailed spatial distributions.

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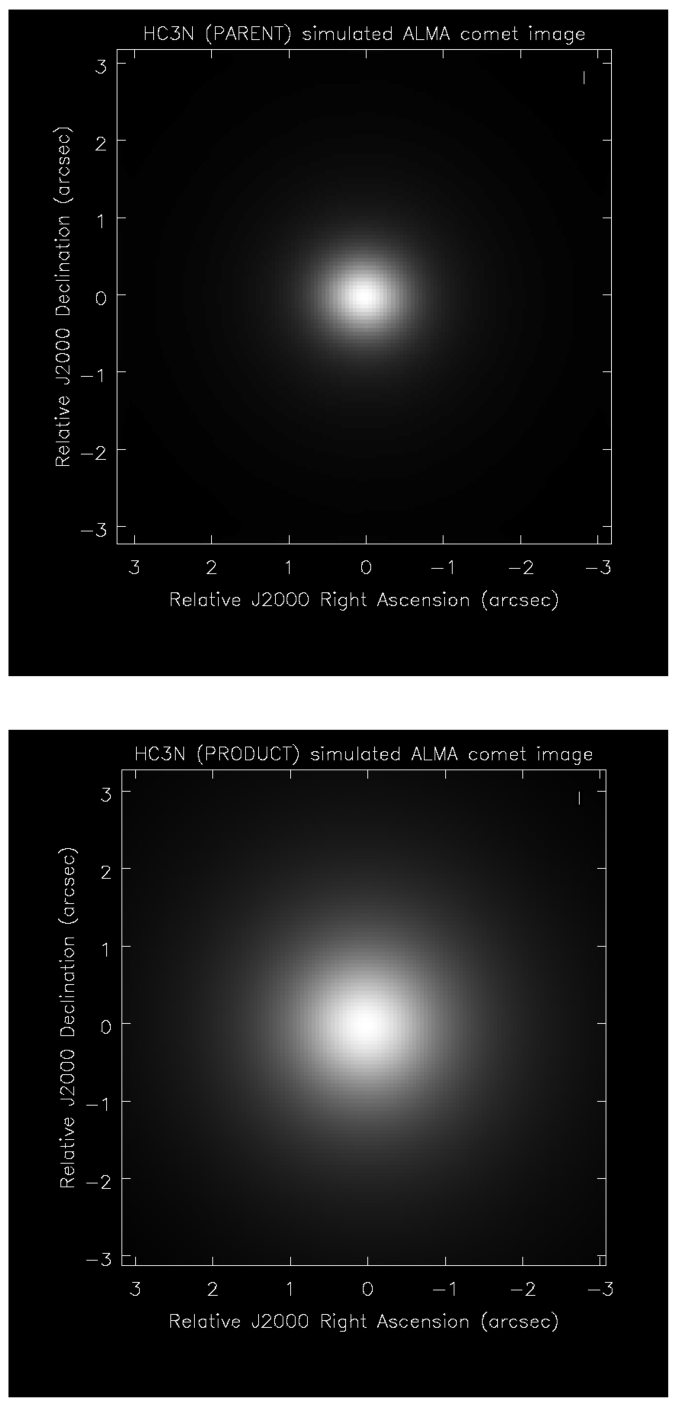

Fig 3: Simulated ALMA images of cometary HC_3N: (top) as a parent molecule, native to the nucleus, and (bottom) as a product species, produced via our chemical scheme. The extent of the distribution reveals the molecule's origin.

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