INVESTIGATING THE SYNTHESIS OF ORGANIC MOLECULES IN COMETARY COMAE VIA NEUTRAL-NEUTRAL REACTIONS. M. A. Cordiner[1,2] and S. B. Charnley[1], [1]Astrochemistry Laboratory, NASA Goddard Space Flight Center, 8800 Greenbelt Road, Greenbelt, MD 20771, USA, [2]Institute for Astrophysics and Computational Sciences, Catholic University of America, 620 Michigan Ave NE, Washington DC 20064, USA.

Introduction: Cometary ices have remained largely unaltered since they accreted during the birth of the planets, so their study provides unique information on the chemical conditions prevalent during the earliest history of our Solar System [1]. Comets are also believed to have delivered volatiles and organics during impacts with planets, so understanding comet compositions provides insight into the chemical regents that may be present to drive prebiotic chemistry on young planetary surfaces [2].

Cometary ice abundances are derived primarily through remote observations of their atmospheres (comae). However, coma mapping observations reveal that some well-known cometary molecules (such as C_2, HNC and H_2CO) originate not from the nucleus, but in the coma, where they are produced as a result of thermal/photochemical processes. It is commonly assumed that other, more complex organic molecules in cometary comae (such as those observed at radio wavelengths) are present in the ice, but this is largely unproven. In fact, our latest chemical/hydrodynamic coma models show that complex organic molecules can be produced in the coma via gas-phase (neutral-neutral) chemistry.

Here we present chemical model calculations for cometary HC_3N and NH_2CHO, demonstrating that coma synthesis is possible for these species.

Chemical Model: Our coma chemical model is based on the original FORTRAN code of Rodgers & Charnley [3], with updated C, N, O chemistry [4]. The gas-phase abundances (n_i) of 280 species, and the temperatures (T_x) of three fluids (ions, neutrals and electrons) are calculated as a function distance (*R)* from the nucleus, and the DVODE package is used to solve the coupled differential equations:

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

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

The source terms N_i are equal to the sum over all chemical production and loss rates for each species (i), v is the coma outflow velocity, T_x, N_x are the respective temperature and density source terms for each fluid (x), γ_x are the ratios of specific heats and G_x are the energy source terms, including energetic contributions due to chemical reactions, collisions between ions, neutrals and electrons, and radiative energy loss from H_2O.

Parent gases are released from the nucleus, undergoing isotropic expansion into the vacuum, and are subject to photolysis by Solar radiation. The ensuing photochemistry is modeled using 3851 reactions involving 101 neutrals, 154 cations and 23 anions. Abundances of parent molecules are for a typical "organic rich" comet [5,6], and we assume a nucleus H_2O production rate of 5×10^{29} mol. s^{-1}. Coma sources of H_2CO and CN are included, consistent with previous observations showing extended spatial distributions for these molecules.

Formamide (NH_2CHO) is produced in the coma by the following neutral-neutral reaction (at a rate calculated by Barone et al. [7]):

$$NH_2 + H_2CO \rightarrow NH_2CHO + H \qquad (1)$$

Cyanoacetylene (HC_3N) production occurs as a result of the reaction (measured in the laboratory by Sims et al. [8]):

$$CN + C_2H_2 \rightarrow HC_3N + H \qquad (2)$$

Results: Our numerical model tracks the coma gas abundances as a function of radius, as shown for several example species in Figure 1. The photolysis of ammonia (NH_3) leads to a large abundance of NH_2 in the coma. This reacts with gas-phase H_2CO to form NH_2CHO. A peak NH_2CHO production rate of 2.3×10^{26} s^{-1} is reached around 620 km from the nucleus. Abundant CN is produced from the photolysis of nitrogen-bearing organics, which reacts with C_2H_2 (sublimated directly from the nucleus) to form HC_3N. The peak HC_3N production rate is 6.4×10^{25} s^{-1} (~2,000 km from the nucleus).

The resulting, beam-averaged NH_2CHO and HC_3N abundances (with respect to H_2O) are within the range of values previously observed in Oort Cloud comets using the IRAM 30-m radio telescope [5]. The predicted abundances for these species are sensitive to assumptions made regarding the coma sources of H_2CO and CN, which will be discussed in more detail in our presentation.

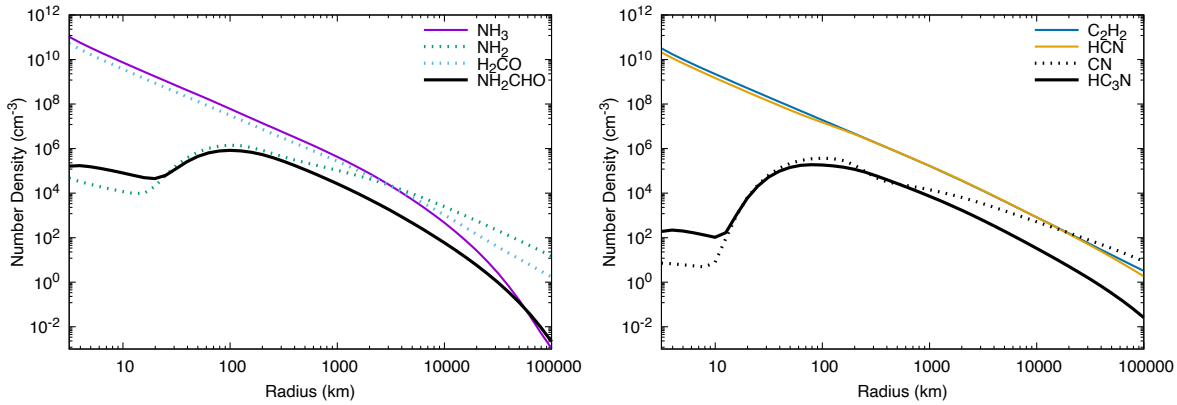

Figure 1: Output from our coma model showing molecular number densities calculated as a function of radius. Coma parent species are shown with solid-colored curves, and photolysis products are shown with dotted line styles (H_2CO is both a parent and a product species). Thick black curves show NH_2CHO (left) and HC_3N (right), formed as a result of Equations (1) and (2), respectively.

Conclusion: Our model shows that both NH_2CHO and HC_3N can be produced in cometary comae through known gas-phase reactions involving simple chemical precursors previously observed to be abundant in comets.

We thus conclude that coma chemistry involving neutral-neutral reactions may be responsible for the synthesis of some of the complex organic molecules observed previously in comets at radio wavelengths.

The proposed coma production mechanisms for HC_3N and NH_2CHO can be tested through interferometric mapping using the Atacama Large Millimeter/submillimeter Array (ALMA), which will be required to reveal, for the first time, the detailed spatial distributions of these molecules and confirm whether or not they are present in ices stored inside cometary nuclei.

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