MODELS FOR COMETARY COMAE CONTAINING NEGATIVE IONS.

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Introduction: The presence of negative ions (anions) in cometary comae is known from Giotto mass spectrometry of 1P/Halley. The anions O^-, OH^-, C^-, CH^- and CN^- have been detected, as well as unidentified anions with masses 22-65 and 85-110 amu [1]. Organic molecular anions such as C_4H^- and C_6H^- are known to have a significant impact on the charge balance of interstellar clouds and circumstellar envelopes and have been shown to act as catalysts for the gas-phase synthesis of larger hydrocarbon molecules in the ISM, but their importance in cometary comae has not yet been fully explored. We present details of our new models for the chemistry of cometary comae that include atomic and molecular anions. We calculate the impact of these anions on the charge balance and examine their importance for cometary coma chemistry.

Method: The coma model is based on the combined chemical and hydrodynamical model of Rodgers & Charnley (2002) [2]. The reaction set has been expanded to include 2977 reactions between 245 chemical species, including chains with up to 6 carbon atoms. Differential equations for the chemical abundances and the energy balance are solved as a function of distance from the cometary nucleus. The model is spherically symmetric and includes the following new anion chemical processes: radiative electron attachment, dissociative electron attachment (DEA), associative electron detachment, photodetachment, collisional charge-transfer, mutual (anion-cation) neutralization, anion-neutral scattering, proton transfer and polar photodissociation (PPD).

Results: Assuming a Halley-like comet (at 0.89 AU with $Q_0 = 6.9\times10^{29}$ mol s^{-1}), carbon-chain-bearing species are produced efficiently in the model coma as a result of acetylene photochemistry. At distances $r \sim 10^4$ km from the nucleus, the model produces peak HC_3N, C_4H and C_4H_2 abundances ~ 0.01% of H_2O (See Figure 1). Hydrocarbon anions are produced predominantly by radiative electron attachment to C_4H and C_6H. The cyanide anion (CN^-) is subsequently produced by transfer of a proton from HCN to the hydrocarbon anions. Other anions are produced in the coma as a result of PPD and DEA, including O^- and OH^-.

If the cometary nucleus contains a sufficient quantity of carbon chains (e.g. C_4H or C_6H, with mixing ratios ~ 10^{-4} – 10^{-3}), rapid radiative electron attachment to these species occurs in the inner coma. This results in reduced abundances of free electrons such that molecular anions can become the dominant carriers of negative charge at $r < 10^3$ km (as shown by comparison of the C_6H^- and e^- profiles in Figure 1). The reduced electron abundance has nuerous effects on the coma physics and chemistry, which will be discussed. For example, the ion temperature in the inner coma (at $r \sim 100$ km), is reduced by a factor of three.

References: [1] Chaizy, P. et al. 1991, *Nature*, 349, 393. [2] Rodgers, S.D. & Charnley, S.B. 2002, *MNRAS*, 330, 660.

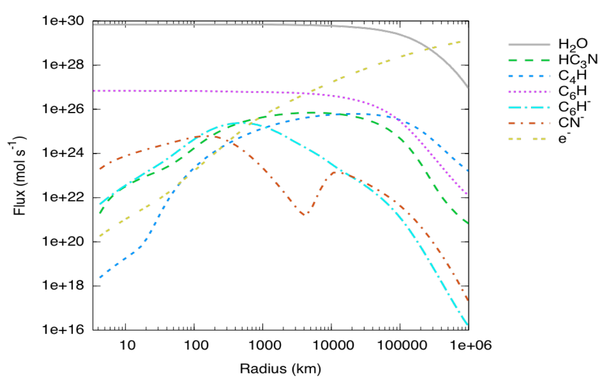

Figure 1. Modeled fluxes of selected species in the coma of a Halley-like comet, as a function of distance from the nucleus. Representative carbon chains and anions are shown, as well as the free electron abundance, the chemical importance of which will be discussed in detail.