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Introduction: Modeling is essential to understand the important physical and chemical processes that occur in cometary comae, especially the relationship between native and sibling molecules, such as, HCN and CN. Photochemistry is a major source of ions and electrons that further initiate key gas-phase reactions, leading to the plethora of molecules and atoms observed in comets. The effects of photoelectrons that react via impacts are important to the overall ionization in the inner coma. We identify the relevant processes in the collision-dominated, inner coma of a comet within a global modeling framework to understand observations of cometary species, especially relationships between native and sibling molecules.

HCN and CN: The CN source(s) must be able to produce highly collimated jets, be consistent with the observed CN parent scale length, and have a production rate consistent with the observed CN production. HCN fulfills these conditions in some comets (e.g., 1P/Halley [1,2], C/2002 T7 (LINEAR) [3], 17P/Holmes [2], 73P/S-W 3 [4], 2P/Encke [5]) while it does not in others [6] (e.g., C/1983 H1 (IAA) [7], C/1995 O1 (Hale-Bopp) [8], C/2001 Q4 [3], 8P/Tuttle [9,10], 6P/d’Arrest [11]). We investigate the chemistry of HCN with our chemical kinetics coma model including a network with other possible CN parents, as well as a dust component that may be a potential source of CN [12,13,14]. It is seen that the major destruction pathways of HCN are via photo dissociation (into H and CN) and protonation with water group ions, primarily, H2O+. We find that HCN “recycles” via protonation reactions with H2O+, H2O2+, OH+, and subsequent dissociative recombination. HCN molecules observed in the coma can consist of those initially released from the nucleus (native) and those that are freshly formed at different locations in the coma via these protonation/dissociation reactions. For a modest production rate comet such as C/2012 F6 (Lemmon) we find that the recycled component is only a few percent of the native component. This doesn’t seem to be enough to reconcile discrepancies between IR and radio observations of HCN or HNC abundances in cometary comae. We continue this study for comet with higher production rates.

Other Molecules: We consider chemical recycling of additional cometary molecules, such as, NH3, H2O, water clusters, and others. We note high-resolution spectral observations of comets show “hot” bands of NH3, water, and others [15]. We search for possible explanations with chemical recycling since dissociative recombination usually leaves the neutral molecule in an excited state that leads to prompt emission.


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