PROSPECTS FOR PHOSPHORUS-BEARING MOLECULES IN COMETARY COMAE. D. C. Boice[1] and A.A. de Almeida[2], [1]Southwest Research Institute, 6220 Culebra Road, San Antonio, TX 78238, dboice@swri.edu; [2]IAG/USP, Department of Astronomy, São Paulo, Brasil, amaury@astro.iag.usp.br.

Introduction: Phosphorus is a key element in all known forms of life and phosphorus-bearing compounds have been observed in space (e.g., [1-4]). Phosphorus is ubiquitous in meteorites, albeit in small quantities, with phosphates being found in stony meteorites and phosphides have been identified in iron meteorites. Phosphorus has been detected as part of the dust component in comet Halley [5] but searches for P-bearing species in the gas phase in comets have been unsuccessful [6]. Based of its moderate cosmic abundance (eighteenth most abundant element, [P]/[N] = 4 x 10^{-3}) and the positive identification of P-bearing species in the interstellar medium (such as, PN, PC, HCP and PO), we would expect simple molecules, diatomics (like PH, PO, PC, PS), triatomics (like HCP and PH_2), and possibly other polyatomics (like phosphine PH_3 and diphosphine P_2H_4), to exist in cometary ices, and hence be released into the gas phase upon ice sublimation. We present results from the first quantitative study of phosphorus-bearing molecules in comets [7] to identify likely species containing phosphorus to aid in future searches for this important element in comets, possibly shedding light on issues of comet formation (time and place) and matters of the prebiotic to biotic evolution of life.

Phosphorus and the Origins of Life: Although phosphorus is relatively rare, it is essential for life! Phosphorus is a key ingredient of metabolic molecules (ATP), cell structure (phospholipids), and replication (backbone of DNA and RNA). The phosphate paradox in the evolution of life can be summarized as extreme stability (~10^8 yrs) versus rapid manipulability (~10^{-3} sec). Since P is present in biomolecules – replication, metabolism, & cell structure, and actively scavenged from the environment by life, then perhaps P was also important in the origins of life on Earth. How is P constrained in this matter? Were there extraterrestrial sources? These are unanswered questions in our quest to understand the origins of life.

Coma Chemistry Modeling: SUISEI, our fluid dynamics model with chemistry of cometary comae [8-12], has been adapted to study this problem. SUISEI produces cometocentric abundances of the coma gas species; velocities of the bulk gas, light atomic and molecular hydrogen with escape, and electrons; gas and electron temperatures; column densities to facilitate comparison with observations; coma energy budget quantities; attenuation of the solar irradiance; and other quantities that can be related readily to observations. We have used a generic volatile composition for the comet nucleus initial conditions, based primarily on the Comet Halley mixing ratios with respect to water [11]. For example, nitrogen is 10 times more depleted with respect to the solar abundance in comets so this has been considered in the coma chemistry in our study. This initial model used phosphine (PH_3) as the phosphorus-bearing parent molecule with a mixing ratio based on the cosmic abundance of phosphorus.

Phosphine Chemistry: Over 100 and gas-phase reactions appropriate for coma chemistry have been collected from databases of NIST, UMIST, and JPL, including photodissociation and photoionization of selected P-bearing molecules [13]. More than 30 P-bearing species were added to the chemical network but many electron impact processes are unknown. The chemistry of phosphine in the inner coma is illustrated in the figure. The major destruction channels are photodissociation and protonation with water-group ions. This leads recycling of PH_3 in the inner coma.

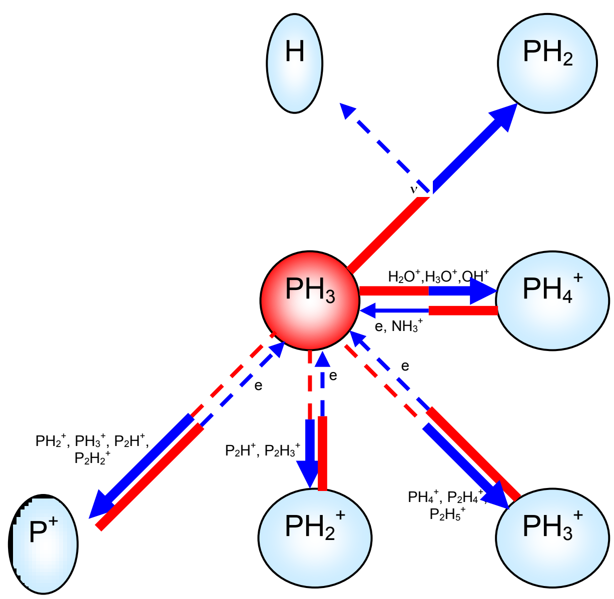

Figure. Relevant coma chemistry for PH_3 in the inner coma. The arrow thickness indicates the importance of the reaction; destruction (red), formation (blue).

Results: PH_3 is a supervolatile, like CO and CO_2. The model chemistry successfully accounts relevant phosphorus chemistry in cometary coma, photo chemistry of PH_3, and other gas-phase reactions. The chemical model can be used to derive abundances of P-bearing species for optical observations and to investigate their chemical pathways in the reaction network as shown in the figure. Initial abundances are found to be on the order of 10^{-4} relative to water, about the same as isotopic species. The scale length of PH_3 in the coma is about 13,000-16,000km. Protonation reactions of PH_3 with water-group ions are important due to the high proton affinity of phosphine. Other P-bearing species likely to be found in the coma include: PH_2, PC, PN, and HCP. Electron impact reactions may also be important but little laboratory data is available. Collaborations with observers to use modern telescopic facilities (e.g., Keck 2 NIRSPEC and Subaru IRCS) are underway to search for the first phosphorus detection in cometary comae.

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