THE COMA CHEMISTRY OF COMET C/2009 P1 (GARRADD). D. C. Boice[1], H. Kawakita[2], H. Kobayashi[2], C. Naka[2], and L. Phelps[3], [1]Southwest Research Institute, 6220 Culebra Road, San Antonio, TX 78238 USA (DBoice@swri.edu), [2]Kyoto Sangyo University, Kyoto 603-8555 Japan, [3]University of Texas at San Antonio, San Antonio, TX USA

Introduction: Modeling is essential to understand the important physical and chemical processes that occur in cometary comae. 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. We identify the relevant processes within a global modeling framework to understand observations of Comet C/2009 P1 (Garradd) and to provide valuable insights into the intrinsic properties of its nucleus. Details of these processes are presented in the collision-dominated, inner coma of the comet to evaluate the relative chemical pathways and the relationship between parent and sibling molecules.

Cometary Processes: Within about 3AU, photochemistry of water is the primary driver of energetics, chemistry, and velocity. Whereas solar visible light mainly heats the nucleus and sublimates volatiles; solar UV initiates photochemistry forming highly reactive ions and radicals that react via gas-phase reactions in the collisionally coupled inner coma. Photo reactions create energetic electrons that cause further ionization via impact reactions. Electron impact processes are very important in moderate to high Q comets [1-4].

Since the temperature of the inner coma gas is very low, electron impact ionization from thermal electrons will not significantly contribute to the overall ionization. However, the average excess electron energy for photoionization of, for example, H_2O in the solar radiation field is of order of 12 to 15 eV depending on solar activity. Thus, secondary ionization from photoelectrons can be important, especially in moderate to high production rate comets. In addition, electrons in the solar wind may contribute to the impact ionization of coma gas. A self-consistent description of the electron energetics and associated processes is necessary to accurately investigate the chemistry in the inner coma: Cometocentric profiles of molecules in the inner coma and mapping the chemical pathways that couple them.

Coma Chemistry Modeling: We have employed a suite of computational tools to analyze observations of Comet C/2009 P1 (Garradd) in order to gain insights into the intrinsic properties of its nucleus and the important physical and chemical processes that occur in the surrounding environment (coma). To obtain the chemical composition by modeling the observed spectra, it is important to take into account all relevant physical and chemical processes with sufficient level of detail that doesn't oversimplify the interpretation of the complex molecular spectra. To this end, we have developed computational tools over the past decades and successfully applied them to comets. The resulting model is versatile and can be applied to *in situ* measurements and observations of comets.

Expected Results: SUISEI, our global fluid dynamics model with chemistry of cometary comae [5-10], has been adapted to study this problem; including, ComChem, a global, gas dynamics simulation with chemistry of the cometary coma, and ComFluo, a time-dependent fluorescence simulation with collisions and superposition of non-equilibrium states appropriate for molecules of interest in comets. 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. Here we describe a systematic study of important cometary molecules in Comet C/2009 P1 (Garradd). Comparisons with high-resolution, near-IR spectra obtained using the NIRSPEC instrument on the Keck 2 telescope taken 31 January 2012 will be made when possible. The combination of these powerful tools results in an innovative and unique opportunity to advance our knowledge of parent molecules in comets, thereby gaining clues to understanding the origins of the solar system and possibly the origins of life on Earth.

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