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Modeling Comet 103P/Hartley 2 for the Deep Impact Extended Investigation (DIXI)

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Abstract

The DIXI mission successfully encountered comet 103P/Hartley 2 on Nov. 4, 2010, and obtained observations using its three scientific instruments. We describe a systematic study of relevant cometary molecules in the coma of comet Hartley 2 relevant to the DIXI encounter. We have employed a suite of computational tools to analyze observations of comet Hartley 2 in order to gain insights into the important physical and chemical processes that occur in its coma and the chemical composition of its nucleus. The computational tools have been developed over the past decades and successfully applied to many comets; including ComChem, a global, gas dynamics simulation with chemistry of the cometary coma and ComFluo, a time-dependent fluorescence model with collisions and superposition of non-equilibrium states appropriate for molecules of interest in comets. 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 details that doesn't oversimplify the interpretation of the complex molecular spectra. The versatile model we have developed accomplishes this and can be applied to *in situ* measurements and observations of other comets and molecules. The model chemistry successfully accounts for composition of many species. For example, the formation of CN is predominately due to photo-dissociation and electron impact dissociation of HCN, but other molecules (e.g., CH_3CN) are minor sources. Cometocentric profiles of other molecules in the inner coma and mapping chemical pathways that couple them are presented.

1. Introduction

Physico-chemical modeling is central to understand the important physical and chemical processes that operate in cometary atmospheres (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 seen in comets. The effects of photoelectrons that react via electron impact reactions are important to the overall ionization. Relevant physico-chemical processes are identified within a global modeling framework to understand observations and *in situ* measurements of comets and to provide valuable insights into the intrinsic properties of their nuclei.

Details of these processes are presented in the collision-dominated, inner coma of comet 103P/Hartley 2; including thermodynamics (e.g., temperature and velocity structure) and photo- and gas-phase chemistry (e.g., composition, gas and electron energetics) throughout this inner region. Prior model results have successfully accounted for the comet Halley water-group composition [1], *in situ* measurements of the PEPE instrument onboard the Deep Space 1 Mission to comet Borrelly [2], S_2 in comet Hyakutake [3], and observations of C_2, C_3, CS, and NS in comet Hale-Bopp [4, 5]. This extensive modeling effort to investigate these important cometary processes is highly relevant to ground-based observations of comets and past, on going, and future spacecraft missions to these primitive objects.

2. 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 high Q comets [4, 6-8].

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 H_2O in the

solar radiation field is about 12 to 15eV, 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.

3. Model Results

Model chemistry successfully accounts for composition of many species. [e.g., HCN and H_2O profiles and C_2 consistency with observations of C_2H_2 and C_2H_6]. The formation of CN is predominately due to photo-dissociation and electron impact dissociation of HCN, but other molecules (e.g., CH_3CN) are minor sources. Dust may also act as a source of CN. The formation of a distributed source of CO at distances throughout the inner coma is due to photo and electron impact reactions of H_2CO and CH_3OH. Uncertainties in reaction rates make this linkage somewhat tentative. The chemical model can be used to derive abundances of C_2H_2, C_2H_6, and C_3H_4 from optical observations of C_2 and C_3 at distances far beyond their direct detection and investigate chemical pathways in the reaction network [4]. Bonev et al. [9] conclude that "Evaluating the relative contributions of these pathways requires further modeling of chemistry," indicating that this study should be continued.

4. Future Work

To extend this study, we plan the following: (1) Cometocentric profiles of other molecules in the inner coma and mapping chemical pathways that couple them, (2) Revise study to incorporate pre-encounter observations of gas and dust to check C_2 and C_3 consistency with observations of C_2H_2 and C_2H_6 [10, 11] and to test conclusions of the present study, (3) Continual updating of chemical reaction network (especially electron impact reactions) and the implementation of rigorous error analysis techniques, (4) Extend study to model post-encounter dynamics and chemistry by developing existing code and to incorporate additional observations of gas and dust to check results.

Acknowledgements

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