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Radial distribution of production rates, loss rates and densities corresponding to ion masses $\leqslant$40 amu in the inner coma of Comet Halley: Composition and chemistry

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Abstract

In this paper we have studied the chemistry of C, H, N, O, and S compounds corresponding to ions of masses $\leqslant$40 amu in the inner coma of the Comet 1P/Halley. The production rates, loss rates, and ion mass densities are calculated using the Analytical Yield Spectrum approach and solving coupled continuity equation controlled by the steady state photochemical equilibrium condition. The primary ionization sources in the model are solar EUV photons, photoelectrons, and auroral electrons of the solar wind origin. The chemical model couples ion–neutral, electron–neutral, photon–neutral and electron–ion reactions among ions, neutrals, electrons, and photons through over 600 chemical reactions. Of the 46 ions considered in the model the chemistry of 24 important ions (viz., $CH_3OH_2^+$, H_3CO^+, NH_4^+, H_3S^+, H_2CN^+, H_2O^+, NH_3^+, CO^+, $C_3H_3^+$, OH^+, H_3O^+, CH_3OH^+, $C_3H_4^+$, $C_2H_2^+$, C_2H^+, HCO^+, S^+, CH_3^+, H_2S^+, O^+, C^+, CH_4^+, C_2^+, and O_2^+) are discussed in this paper. At radial distances $<$1000 km, the electron density is mainly controlled by 6 ions, viz., NH_4^+, H_3O^+, $CH_3OH_2^+$, H_3S^+, H_2CN^+, and H_2O^+, in the decreasing order of their relative contribution. However, at distances $>$1000 km, the 6 major ions are H_3O^+, $CH_3OH_2^+$, H_2O^+, H_3CO^+, $C_2H_2^+$, and NH_4^+; along with ions CO^+, OH^+, and HCO^+, whose importance increases with further increase in the radial distance. It is found that at radial distances greater than $\sim$1000 km ($\pm$500 km) the major chemical processes that govern the production and loss of several of the important ions in the inner coma are different from those that dominate at distances below this value. The importance of photoelectron impact ionization, and the relative contributions of solar EUV, and auroral and photoelectron ionization sources in the inner coma are clearly revealed by the present study. The calculated ion mass densities are compared with the Giotto Ion Mass Spectrometer (IMS) and Neutral Mass Spectrometer (NMS) data at radial distances 1500, 3500, and 6000 km. There is a reasonable agreement between the model calculation and the Giotto measurements. The nine major peaks in the IMS spectra between masses 10 and 40 amu are reproduced fairly well by the model within a factor of two inside the ionopause. We have presented simple formulae for calculating densities of the nine major ions, which contribute to the nine major peaks in the IMS spectra, throughout the inner coma that will be useful in estimating their densities without running the complex chemical models.

Keywords: Comets, Halley; Ionospheres; Abundances, atmospheres; Photochemistry

1. Introduction

The study of cometary composition has been the subject of great interest since 1986 when High Intensity Ion Mass Spectrometer (HIS-IMS), Neutral Mass Spectrometer (NMS), and Positive Ion Cluster Composition Analyzer of Reme Plasma Analyzer (PICCA-RPA) onboard Giotto

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spacecraft measured a large number of peaks between 12 and 120 amu in the mass spectra of Comet 1P/Halley (Balsiger et al., 1986; Krankowsky et al., 1986; Mitchell et al., 1987). After the encounter of Comet Halley, several theoretical models have been constructed describing the chemistry of cometary coma. But most of these models were limited to the chemistry of only few ions. Allen et al. (1987) derived the concentration of NH_3 and CH_4, relative to H_2O, by fitting the variation with distance of Giotto IMS data. These authors showed that the measured ionosphere profiles were incompatible with pure H_2O coma, and require 1–2% NH_3. The magneto-hydrodynamic–chemical model of Wegmann et al. (1987) (cf., also Schmidt et al., 1988) also yielded similar results. Marconi and Mendis (1988) reanalyzed the IMS data and found that an enhancement of solar EUV flux, responsible for ionization, can also account for the IMS observations.

Boice et al. (1990) suggested that most of the CH_4 estimated using the IMS data is not from volatiles released directly from the nucleus but is a by-product of polyoxymethylene (POM), a constituent of the complex organic mixture in CHON particle (Huebner et al., 1989). Boice et al. derived an upper limit of 0.5% for the ratio of CH_4/CO. However, Wegmann et al. (1987) did include 3% POM in their model, and found that the data of IMS for singly charged ions with masses from 6 to 20 amu were in better agreement by including POM in the model than by excluding POM, but requires about 2% CH_4 in the nucleus. Ip et al. (1990) derived the relative abundance of HCN of 0.02% using a photochemical model and fitting the IMS data peak at 28 amu. Two sharp peaks observed in the PICCA data at 37 and 39 amu are identified as the organic ions C_3H^+ (Marconi et al., 1989) and $C_3H_3^+$ (Korth et al., 1989), respectively, whose sources are attributed to the circum-nuclear distribution of the CHON dust particles observed at the comet.

Geiss et al. (1991) reported that the IMS data between masses 25 and 35 amu are dominated by H_3CO^+ and $CH_3OH_2^+$, which give rise to peaks in the IMS data at 31 and 33 amu. Marconi et al. (1991) studied the chemistry of sulfur ions H_3S^+, HCS^+, H_3CS^+, and SO^+ corresponding to masses 35, 45, 47, and 48 amu, respectively, in the PICCA data. They have argued that H_3S^+ is a dominant ion in the chemistry of sulfur group ions, whose likely parent molecule is H_2S (Marconi et al., 1990). Mitchell et al. (1992) extended the analyses of Giotto PICCA data to higher masses. Meier et al. (1993) analyzed Giotto NMS data and found that the peak at 31 amu is dominated by protonated formaldehyde ion H_3CO^+, and that most of the H_2CO comes from an extended source; the data can be reconciled even if H_2CO is not a parent molecule that evaporates from the nucleus. Eberhardt et al. (1994) also suggested that the mass channels at 33 and 35 amu are dominated by methanol and hydrogen sulfide, respectively, and derived their relative abundances on the Comet Halley.

Haider et al. (1993) solved coupled continuity equations for chemical steady state conditions using the chemistry of H_2O, NH_3, and CH_4. In this paper, the ratios of masses 19/18, 17/19, and 15/19 were determined and compared with Giotto IMS data to derive the abundances of NH_3 and CH_4 in the coma of Comet Halley, which were about 1.5% NH_3 and 0.5% CH_4. Meier et al. (1994) also derived the abundance of ammonia using the NMS data and found results similar to those of Haider et al. (1993). Altwegg et al. (1994) analyzed the IMS-HIS data and reported that in the group of masses 12–16 amu the most abundant ion is CH_3^+ whose parent molecule could be CH_2. Haberli et al. (1995) developed a chemical-transport model to investigate the cause of sharp enhancement in ion density observed by Giotto IMS at a cometocentric distance of about 12,000 km, by incorporating the chemistry of 5 major parent species in the model. Detailed analysis of the distribution of H_2O^+ ions in the coma of Comet Halley has also been attempted recently using the MHD model with chemistry (Haberli et al., 1997; Wegmann et al., 1999). The study of Wegmann et al. (1999) suggested that about 3% of H_2O is finally converted to H_2O^+ on Comet Halley.

Bhardwaj et al. (1996) developed a coupled chemistry-transport model to study the chemistry of atomic carbon and oxygen in the inner coma of Comet Halley. Their calculations revealed that the electron impact dissociation of parent species could be a potentially important source of C and O production and their emissions in the inner cometary coma. Later this calculation was expanded, and extended to investigate the chemistry of $C(^1D)$ atom and the mechanisms of generation of CI 1931 Å emission (Bhardwaj, 1999) in the inner coma of Comet Halley, and the production of $O(^1D)$ atom and OI 6300 Å emission (Bhardwaj and Haider, 2002) on Comet Wirtanen.

2. Objective

The objectives of this paper are: (1) to study the chemistry of C, H, N, O, and S compounds corresponding to mass of ions $\leqslant$40 amu observed by HIS sensor of the Giotto IMS experiment in the inner coma ($\leqslant 10^4$ km) of Comet Halley, and (2) to investigate how the different sources of ionization, viz., solar EUV photons, photoelectrons and auroral electrons of solar wind origin, play their role in different physical and chemical processes in the coma, and thereby affecting the production and density of these ions. The chemical modeling of all ionic species corresponding to 10–120 amu is very difficult because of rapidly increasing number of possible species at larger masses. Already more than 22 molecules have now been identified as parent molecules outgassing from the nucleus (e.g., Crovisier, 1999). Moreover, several molecular and atomic species have been spectroscopically detected in the cometary coma at UV, visible, IR, and radio wavelengths. Although a few of these are simple parent molecules (i.e., H_2O, CH_4, CO, CO_2, N_2, HCN, H_2CO, CH_3OH, NH_3, SO_2, H_2CS, CS_2), most are radicals and ions that appear to be dissociation fragments of more complex, but unknown species. These molecules need not sublime