

ON THE RELATIONSHIP OF CHEMICAL ABUNDANCES IN THE NUCLEUS TO THOSE IN THE COMA

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Abstract. One of the goals of comet research is the determination of the chemical composition of the nucleus because it provides us with the clues about the composition of the nebula in which comet nuclei formed.

It is well accepted that photo-chemical reactions must be considered to establish the abundances of mother molecules in the coma as they are released from the comet nucleus or from distributed dust sources in the coma. However, the mixing ratios of mother molecules in the coma changes with heliocentric distance. To obtain the abundances in the nucleus relative to those in the coma, we must turn our attention to the release rates of mother molecules from the nucleus as a function of heliocentric distance. For this purpose, we assume three sources for the coma gas: the surface of the nucleus (releasing mostly water vapor), the dust in the coma (the distributed source of several species released from dust particles), and the interior of the porous nucleus (the source of many species more volatile than water). The species diffusing from the interior of the nucleus are released by heat transported into the interior. Thus, the ratio of volatiles relative to water in the coma is a function of the heliocentric distance and provides important information about the chemical composition and structure of the nucleus.

Our goal is to determine the abundance ratios of various mother molecules relative to water from many remote-sensing observations of the coma as a function of heliocentric distance. Comet Hale-Bopp is ideal for this purpose since it has been observed using instruments in many different wavelength regions over large ranges of heliocentric distances. The ratios of release rates of species into the coma are then modeled assuming various chemical compositions of the spinning nucleus as it moves from large heliocentric distance through perihelion. Since the heat flow into the nucleus will be different after perihelion from that before perihelion, we can also expect different gas release rates after perihelion compared to those observed before perihelion. Since not all the data are available yet, we report on progress of these calculations.

Keywords: Comet nucleus, coma, volatile ices

1. Introduction

The structure and composition of comet nuclei provide information about the nebula in which comets formed: they reflect the chemical composition of the nebula, the thermodynamic conditions in the nebula, and the physical accretion processes.



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Observations of the coma yield only indirect information about mother molecules and atoms (such as H_2O , HCN , H_2CO , NH_3 , CH_3OH , CH_4 , CO , CO_2 , C_2H_2 , C_2H_6 , Na , and others), molecular radicals (such as C_2 , C_3 , NH , NH_2 , OH , S_2 , and others), and ions (such as H_2O^+ , H_3O^+ , NH_4^+ , HCO^+ , CO^+ , CO_2^+ , and others).

To get the composition of the coma at its interface with the nucleus, we must consider photolytic reactions including photodissociation, photoionization, electron collisional dissociation, electron collisional ionization, charge exchange reactions, and protonization reactions. We must also consider the kinetics of the coma gas and its coupling to the dust and the kinetics of chemical reactions. Finally we must consider the solar wind interaction coupled to photolytic processes and in particular energetic reactions.

The chemical species at the coma - nucleus interface are the same as in the comet nucleus. However, the abundances in the coma are not the same as in the comet nucleus. This is immediately clear from the mixing ratio of $\text{CO}/\text{H}_2\text{O}$ in the coma, which changes with heliocentric distance r . The concept of chemical differentiation of the nucleus emerged gradually from heat and gas diffusion models of the nucleus – see, for example, Tancredi et al. (1994) andENZIAN et al. (1997). The differences in the abundance ratios in the coma relative to those in the nucleus were specifically mentioned by EpINASSE et al. (1991); Benkhoff and Huebner (1995) and de Almeida et al. (1996); the latter also pointed out the three sources for the coma gas:

1. The surface of a comet nucleus which provides mostly H_2O and dust.
2. The dust entrained by the escaping gases from the nucleus is distributed throughout the coma and gives rise to some organic species released from hydrocarbon polycondensates in the dust and possibly additional water that was trapped in grain aggregates in the nucleus. We refer to this source as the distributed source.
3. The interior of the nucleus, which provides gases that diffuse through the porous nucleus after being liberated by heat conducted to ices more volatile than water (e.g., CO , CO_2 , CH_3OH , NH_3 , etc.).

The mixing ratio as function of r is the subject of this investigation. Comet Hale–Bopp, which was observed from large heliocentric distances before perihelion to large heliocentric distances after perihelion, is ideally suited for this purpose. Our plan is to start with the simplest calculations and add more complex issues only when needed.

2. Observational Data

We compare our model calculations first with pre-perihelion observational data taken from Schleicher et al. (1997) for H_2O in the visible, Weaver et al. (1997) for H_2O in the UV, and Biver et al. (1997) for H_2O and CO in the radio range of the spectrum. Since the H_2O observational data come from various instruments in different wavelength ranges that are not normalized with each other, we fit these

data to a theoretical H₂O release rates curve and then use this curve in our analysis. No theoretical curve exists for CO released from the interior of the nucleus. Thus, we use a linear regression of the CO observational data to simplify the analysis, but also keep the individual points. The solid line in Figures 1 and 2 is the ratio of the fitted data of CO and H₂O. The black squares are the ratio of the individual observational data points of CO to the fitted data of H₂O.

3. Model Calculations

The computer model that we use has been described by Benkhoff and Huebner (1995). We assume a comet nucleus in the orbit of Comet Hale–Bopp with semi-major axis $a = 185.55$ AU, eccentricity $e = 0.99507$, spin axis perpendicular to the orbit plane, and a spin period $P_s = 12^h$. Calculations were started with the model comet at $r = 28$ AU, pre-perihelion, and ended at 1.7 AU, post-perihelion. However, we report only on the pre-perihelion calculations in the range where observational data are available.

We assume an albedo of 4% and an IR emissivity of 96%. The starting temperature in the nucleus was 10 K. The initial porosity was $\psi = 0.5$, tortuosity $\tau = 1.5$, conductivity of crystalline ice $\kappa_c = 567/T \text{ Wm}^{-1} \text{ K}^{-1}$, conductivity of amorphous ice $\kappa_a = 7.1 \times 10^{-7} T \text{ Wm}^{-1} \text{ K}^{-1}$, conductivity of dust $\kappa_d = 40 \text{ Wm}^{-1} \text{ K}^{-1}$, and the effective conductivity was $\kappa_i^{\text{eff}} = h\kappa_i$. Here h is the Hertz factor.

The parameters we explore are the Hertz factor for the conductivity of the matrix materials, the pore size, and the relative abundances of CO and H₂O of the nucleus. We also consider mixtures with and without dust. H₂O ice may be crystalline or amorphous. CO can exist either as a frozen gas or trapped in the matrix of the amorphous H₂O ice.

We have varied the pore radius from 1 mm to 1 cm, the Hertz factor from 10^{-4} to 10^{-2} , and the composition, including the ice to dust ratio. The CO abundance in the ice was varied from 10% to 25% by mass and the H₂O abundance in the ice correspondingly from 90% to 75%.

4. Results

In Figures 1 and 2 we show a very limited number of results from the many parameter studies we have made. Figure 1 shows results for crystalline water ice and Figure 2 for amorphous water ice. In neither calculation was CO trapped in the ice. The presence of dust reduces the water release and thus raises and flattens the mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ at small r .

1. The mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ in the coma for some dust-free mixtures of CO and crystalline H₂O ice agree reasonably well with observations at large heliocentric distances ($r > 3$ or 4 AU, depending on the mixture) but are always too low at small r .

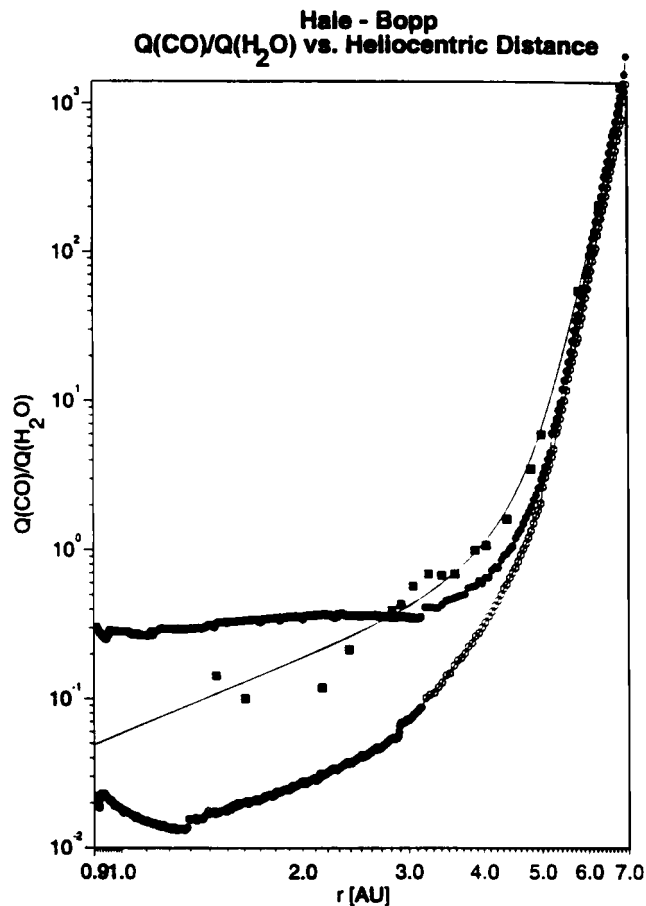


Figure 1. Mixing ratio of CO/H₂O as a function of heliocentric distance, r , for CO and crystalline water ice with dust (●) and without dust (○) from model calculations. The solid line is the ratio of the fitted data of CO and H₂O from observations. The black squares are the ratio of the individual observational data points of CO to the fitted data of H₂O.

2. The mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ in the coma for a dusty nucleus with CO and crystalline H₂O ice is very flat at small heliocentric distances ($r < 3$ AU) and too low in the range from $r = 3$ AU to 5 AU.

3. The mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ in the coma for some dust-free mixtures of CO ice and amorphous H₂O ice are similar to those with crystalline H₂O ice, but do not fit as well at large heliocentric distances ($r > 6$ AU). In this model we assumed that CO may have recondensed in the outer layers of the nucleus after perihelion passage of a previous orbit. Thus, we assumed that the CO was not trapped in the amorphous H₂O ice. (The undulations at small r were caused by an instability in the computer program.)

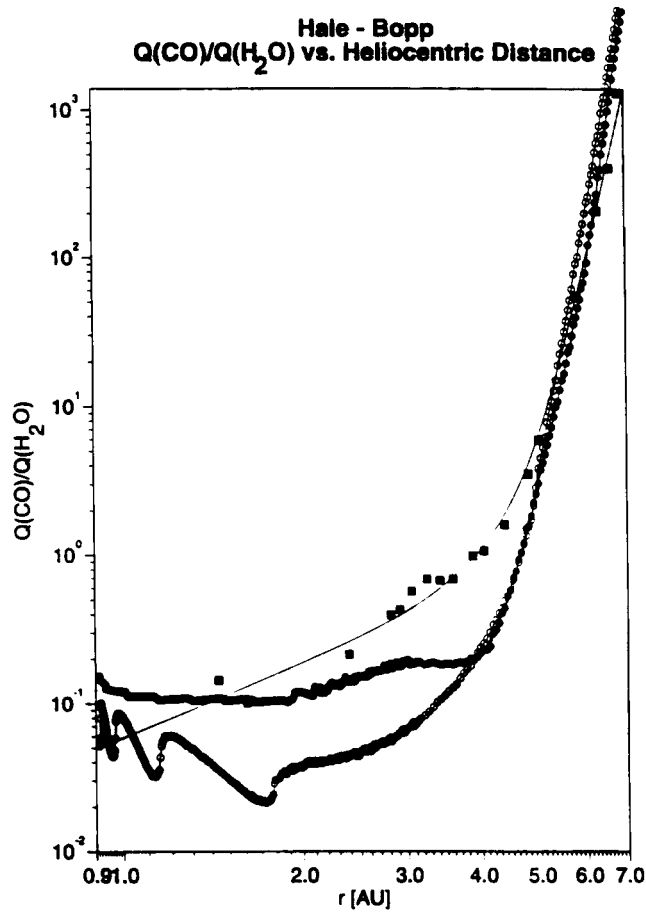


Figure 2. Similar to Figure 1, except for amorphous water ice.

4. The mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ in the coma for a dusty nucleus with CO and amorphous H_2O ice show the best agreement below $r = 3$ AU. As in (3), we assumed that the CO was not trapped in the amorphous H_2O ice.

5. Conclusions

As can be seen from Figures 1 and 2, the observed mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ is bracketed by model calculations with and without dust in most, but not all regions. Results are sensitive to the Hertz factor, pore radius, and the composition. Thus some information about the composition in the cloud in which comets formed and the physics of the accretion processes may be attainable from analyses as suggested here.

The mixing ratios of $Q(\text{CO})/Q(\text{H}_2\text{O})$ in the coma for some dust-free and dusty mixtures with CO *trapped* in amorphous H_2O ice still need to be investigated. The distributed sources, mentioned earlier, have not been included as yet. They may change the $Q(\text{CO})/Q(\text{H}_2\text{O})$ ratio by about a factor of two at small heliocentric distances where dust disintegration is more likely. More data, particularly from post-perihelion observations will be needed for such an analysis. We also expect the mixing ratio of $Q(\text{CO})/Q(\text{H}_2\text{O})$ to change as we add other species to the model calculations. The latent heats of the volatile species that we will consider lie between those of H_2O and CO and thus will influence the temperature gradient into the nucleus and the amount of heat reaching the CO sublimation front.

Acknowledgements

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