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The Contribution of Electron Collisions to Rotational Excitations of Cometary Water

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Abstract

The e-H_2O collisional rate for exciting rotational transitions in cometary water is evaluated for conditions found in comet Halley during the Giotto spacecraft encounter. In the case of the $0_{00} \rightarrow 1_{11}$ rotational transition, the e-H_2O collisional rate exceeds that for excitation by neutral-neutral collisions at distances exceeding 3000 km from the cometary nucleus. Thus, the rotational temperature of the water molecule in the intermediate coma may be controlled by collisions with electrons rather than with neutral collisions, and the rotational temperature retrieved from high resolution infrared spectra of water in comet Halley may reflect electron temperatures rather than neutral gas temperature in the intermediate coma.

1 Introduction

The encounters of the Giotto and Vega spacecraft with comet Halley, and observations with space-based (IUE), airborne (KAO), and ground-based telescopes, during Halley's last apparition resulted in major advances in our understanding of its chemical composition and of the physical conditions and physical processes in the cometary coma. While *in situ* measurements provided direct information on conditions in the intermediate coma during the spacecraft encounters, it is the earth-based spectroscopy of parent molecules, especially water vapor (the dominant volatile species in the comet), that offers a remote but direct probe of physical conditions there. However, these conditions may only be retrieved from spectral data if the processes that control rotational populations and spectral line formation are well understood. The theoretical studies by Bockelee-Morvan (1987) and Storrs and Mumma (1991) achieved satisfactory fits to the line-by-line intensities revealed in infrared spectra of the ν_3-band of water in comet Halley acquired on the Kuiper Airborne Observatory (KAO) (Mumma et al. 1986 and Weaver et al. 1987). However, the use of a cross-section of $5 \times 10^{-14} cm^2$ or larger is questionable. Storrs and Mumma (1991) suggested the need for such a large cross-section could indicate that other processes, such as electron or ion collisions, were affecting rotational excitations. High electron density deduced from Giotto and Vega measurements (Ip and Axford 1990, Pedersen et al. 1987) and low electron temperature in the inner coma from the ionosphere model (Körömezey et al. 1987) could make electron collisions non-negligible in exciting water rotational transitions.

2 Collisional cross-sections for water rotational transitions

Itikawa (1972) used the Born approximation to calculate the cross-section for rotational transitions by $e - H_2O$ collisions, which cross-section is formulated as follows

$$\sigma_{J_{K_a K_c} \rightarrow J'_{K'_a K'_c}} = \frac{8\pi}{3k^2} \frac{D^2}{2J+1} S_{J'_{K'_a K'_c} J_{K_a K_c}} \ln \frac{k+k'}{k-k'}, \tag{1}$$

where D=1.85 Debye is the permanent dipole moment of the water molecule; J, K_a and K_c are quantum numbers for the initial state of the transition and J', K'_a and K'_c for the final state; and k and k' are the

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initial and final wave numbers of the electron. The line strength $S_{J'_{K'_a K'_c} J_{K_a K_c}}$ is given in Schwendeman and Laurie (1958). In the paper by Xie and Mumma (1992), it is shown that the calculated cross-sections from Eq (1) are consistent with the total cross-section measurements from the electron scattering experiments at low impact energy by Sokolov and Sokolova (1982), and the effective $H_2O - H_2O$ cross-section is probably far smaller than $5 \times 10^{-14} cm^2$ currently used in the literature. In our evaluation, the H_2O-neutral gas cross-section is taken to be $5 \times 10^{-14} cm^2$, which is the upper limit.

3   Collisional rate for the $0_{00} \rightarrow 1_{11}$ rotational transition

The electron temperature is relatively low with $T_e < 300K$ and follows the neutral gas temperature inside the contact surface (Körömezey et al. 1987), it increases with cometocentic distance outside the contact surface (Gan and Cravens 1990), where electron heat conduction becomes important. In our evaluation, the electron temperature in the cometary coma is taken to be approximately equal to the ion temperature measured from Giotto (Lämmerzahl et al. 1987).

$$
T_e = \begin{cases}
200 \ K & r < 4500km \\
2000 \ K & 4500km < r < 7280km \\
5000 \ K & 7280km < r < 1.25 \times 10^4 km \\
10000 \ K & 1.25 \times 10^4 km < r < 2 \times 10^5 km
\end{cases} \tag{2}
$$

The electron density is assumed to be equal to the total ion density from Giotto measurements (after Ip and Axford 1990) as follows

$$
n_e = \begin{cases}
\frac{1.3 \times 10^7}{r} \ cm^{-3} & r < 7280km \\
1.7 \times 10^{-2} r^{1.3} \ cm^{-3} & 7280km < r < 1.25 \times 10^4 km \\
5.6 \times 10^3 (\frac{10^4}{r})^2 \ cm^{-3} & 1.25 \times 10^4 km < r < 2.0 \times 10^5 km,
\end{cases} \tag{3}
$$

where r is the cometocentric distance in km. The corresponding H_2O production rate at the Giotto encounter was about 5×10^{29} molecules/sec (Krankowsky et al. 1986). The collisional excitation rate (s^{-1}) for the rotational transition $0_{00} \rightarrow 1_{11}$ is given in the following form

$$
\nu_{e-H_2O} = \begin{cases}
\frac{29}{r} \ s^{-1} & r < 4500km \\
\frac{18}{r} \ s^{-1} & 4500km < r < 7280km \\
1.7 \times 10^{-8} r^{1.3} \ s^{-1} & 7280km < r < 1.25 \times 10^4 km \\
45 \times (\frac{10^2}{r})^2 \ s^{-1} & 1.25 \times 10^4 km < r.
\end{cases} \tag{4}
$$

The corresponding water-neutral gas collision frequency at cometocentric radius r is given by

$$
\nu_{H_2O - H_2O} = \frac{7.5 \times 10^4}{r^2} s^{-1}. \tag{5}
$$

Here the expansion velocity of the neutral gas is taken as 1.0 km/s and kinetic temperature of water molecules is 60 K in the coma a few thousand kilometers away from the nucleus.

4   Rotational populations of water molecule in Comet Halley

The excitation rate for the $0_{00} \rightarrow 1_{11}$ transition is shown in Fig. 1a . It is clear that for the $0_{00} \rightarrow 1_{11}$ transition the $e - H_2O$ collisional excitation rate will be equal to that of $H_2O - H_2O$ collisions somewhere around $10^3 - 10^4 km$ and will exceed the latter in the more distant region. The excitation rate due to vibrational infrared fluorescence (at 0.9 AU) is also plotted in Fig. 1a. Clearly infrared resonance fluorescence dominates rotational pumping only in the outer coma. De-excitational rates for the $0_{00} \rightarrow 1_{11}$ rotational transition are shown in Fig. 1b , where the rates for relaxation by $e - H_2O$ and $H_2O - H_2O$ collisions are compared with radiative relaxation in the optically thin case. In the optically thick coma,

optical trapping leads to an efficient reduction in the Einstein-A coefficient and enhances the effect of collisions (Xie and Mumma 1992). For the active comet with a gas production rate of $5 \times 10^{29} mol/s$, the critical radius corresponding to $r_c = 1.0$ is about 1×10^5 km for the $0_{00} \rightarrow 1_{11}$ rotational transition. The intermediate coma ($r \leq\sim 1 \times 10^4$ km) sampled by the KAO observations is optically thick for the $0_{00} \rightarrow 1_{11}$ rotational transition. As the result of optical trapping, there is a more extended inner coma, where collisional relaxation dominates and rotational excitation for cometary water is controlled by collisional effects, not by fluorescence. In the region where the electron collisional rate is comparable to or larger than that of neutral gas collisions, electron collisions will affect the rotational population. Therefore, the temperature measured for the rotational states will be a measure of the electron or neutral kinetic temperatures, depending on cometocentric distance. In the intermediate region, where electron collisions dominate, the rotational temperature is undoubtedly controlled by electrons.

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FIG. 1a   RADIAL DISTANCE(km)

FIG. 1b   RADIAL DISTANCE (km)