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VELOCITY DISTRIBUTIONS OF H AND OH PRODUCED THROUGH SOLAR PHOTODISSOCIATION OF H_2O

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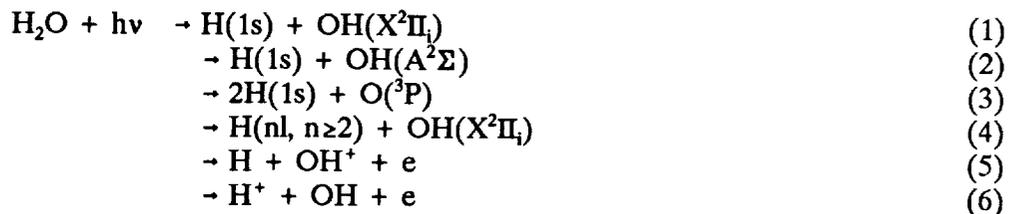Los Angeles, CA 90089-1341

The calculated velocity distributions of atomic hydrogen and hydroxyl radicals produced through solar photodissociation of gaseous water molecules are presented. Under collisionless conditions, the calculation has been carried out using the most recent available data for the production of H and OH through photodissociation of H_2O from its dissociation onset throughout the EUV region. Because the lack of data in certain spectral regions, we can only obtain an upper and lower bounds to the velocity distributions. The results show that the H atoms and OH radicals produced exhibit multiple velocity groups. Since most of the current cometary modeling uses a single velocity of 20 km/s associated with the photodissociation of H_2O, the present results may be useful in interpreting the *many peaks* observed in the velocity distributions of cometary atomic hydrogen.

INTRODUCTION

H_2O is a major constituent of the atmospheres of comets, satellites of the outer solar system, and is also a major constituent of the atmosphere of the Earth. A major feature of comets is the extended atomic hydrogen coma which can reach tens of gigameters (10^6 km) from the nucleus. Observations of atomic hydrogen emission lines (Ly-α; Ly-β; and Hα) yield information about the heliocentric variation of the total gas production rate, since H_2O is apparently the ultimate parent of H. Such data also provide information about the hydrogen velocity distribution, the lifetime of atoms against solar wind charge exchange and photoionization loss, and the solar Ly-α radiation pressure. Similarly, observations of the 18-cm OH line profiles have yielded information on the velocity distributions of the ejected OH and on the expanding cometary H_2O.

The hydrogen Ly-α isophotes in the outer region observed in several comets can be reproduced by a theoretical model assuming a two-component (20 and 8 km/s) Maxwellian velocity distribution of H atoms with equal production rates. It has been suggested that the high-velocity component arises from photodissociation of H_2O and the low-velocity component from photodissociation of OH. A better knowledge about the velocity distribution of H atoms and OH radicals produced through photodissociation of H_2O can be obtain in a more rigorous treatment of this important problem. Such a velocity distribution can in principle be determined if the partial cross sections of *all* the possible photodissociation processes are known.

The relevant processes that produce H and OH photofragments in the ground and excited states are:

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\begin{aligned}
H_2O + h\nu \quad &\rightarrow H(1s) + OH(X^2\Pi_i) & (1)\\
&\rightarrow H(1s) + OH(A^2\Sigma) & (2)\\
&\rightarrow 2H(1s) + O(^3P) & (3)\\
&\rightarrow H(nl,\ n\geq2) + OH(X^2\Pi_i) & (4)\\
&\rightarrow H + OH^+ + e & (5)\\
&\rightarrow H^+ + OH + e & (6)
\end{aligned}
$$

In his pioneering work, *Festou* [*1981*] only treated process (1) and only considered the first absorption band of H_2O in the 1360-1860 Å region and the absorption at the H Ly-α line. Recently, *Crovisier* [*1989*] improved the model calculation by including the vibrational energy distributions of the ground state OH fragment and obtained an averaged OH velocity of 1.05 km/s (the corresponding H velocity is 17.85 km/s). This velocity is 10% smaller than that derived by neglecting the internal vibrational energy of $OH(X^2\Pi_i)$ photofragments. In the present work we have extended the photon wavelength from 1860 Å throughout the EUV region and have also included the six photodissociation processes listed above.

TOTAL AND PARTIAL PHOTOEXCITATION CROSS SECTIONS OF H_2O

The photoexcitation processes of H_2O in the VUV-EUV region have been extensively studied both experimentally and theoretically [*Dutuit et al., 1985; Wu and Judge, 1988; 1991*] and the photoabsorption and photoionization cross section data are well known. However, only limited photodissociation data are available at a few incident photon wavelengths [*Berkowitz 1979*].

It is well known that photoexcitation of the H_2O molecule rarely results in fluorescence from excited states of the neutral H_2O molecule and parent H_2O^+ ion. In contrast with these, the fluorescence from excited H* and OH* photofragments is intense, with a maximum quantum yield of 0.12 and 0.1, respectively. In addition to the excited photofragments, the other neutral products may include the parent molecule and neutral photofragments which are in the ground and metastable states. The maximum quantum yields for producing the neutral products [*Wu and Judge 1988*] are 1.0, ~0.6, and ~0.3 for the wavelength ranges >984, 800-984, and 600-800 Å, respectively. By subtracting the partial cross sections for producing the excited photofragments from that of the total neutral products, the remaining cross sections are the cross sections for producing the *undetected* neutral products. The quantum yield for the undetected neutral products can be as high as 0.43 at 810 Å [*Wu and Judge, 1988; 1991*]. In the present work, a lower bound is set for the case that all the *undetected neutral products* are something other than H and OH fragments. An upper bound is set by assuming the *undetected neutral products* are all H and OH fragments. As a result, an upper and lower bounds of velocity distributions are calculated. The *real* distributions will probably lie in between these two extremes.

VELOCITY DISTRIBUTIONS OF DISSOCIATION FRAGMENTS

The excess excitation energy ΔE is defined as the difference between the incident photon energy $h\nu$ and the threshold energy $E_0(\Lambda)$ for the dissociation process of interest at a given temperature, less the internal energy $E(v,J)$, i.e., the vibrational and rotational energies, of the photofragments. This can be expressed as $\Delta E = h\nu - E_0(\Lambda) - E(v,J)$, where Λ is the specific electronic state of the parent molecule involved in the dissociation channel of interest. The v and J are the vibrational and rotational quantum numbers, respectively. From the conservation of energy and momentum the excess energy is converted into kinetic energy of the H and OH fragments in the dissociation of H_2O. The kinetic energy of the respective H and OH fragments is $(17/18)\Delta E$ and $(1/18)\Delta E$. Thus, the velocity of the respective H and OH is $13.44(\Delta E)^{1/2}$ and $0.796(\Delta E)^{1/2}$ km/s with ΔE in units of eV.

The production rate of a specific photofragment is $A(\lambda) = F_{\odot\lambda}\eta_\lambda (1 - e^{-n\ell\sigma})$, where $F_{\odot\lambda}$ is the solar flux at λ, η_λ is the quantum yield for producing the specific photofragments, $n\ell$ is the column density, and σ_λ is the photoabsorption cross section at λ.

The calculation has been carried out using (a) the most recent available absolute absorption cross section of H_2O and the quantum yields for the production of H and OH through photodissociation of H_2O from its absorption onset throughout the EUV region [*Judge and Wu*,

1990; Lee and Suto, 1986; Wu and Judge, 1988; 1991], (b) the newly available vibrational and rotational energy distributions of both the excited [*Lee et al., 1978; Wu and Judge, 1991*] and the ground state [*Engel et al., 1988*] OH photofragments, and (c) the integrated solar flux in 10 Å increments from 500 to 1860 Å in the *continuum* regions [*Lean, 1987; Mount and Rottman, 1983a; 1983b; Valley, 1966*] and the specific wavelength and flux at the bright solar lines [*Valley, 1966*], e.g., the H Ly-α, -β, -γ, O VI, C III, He I, etc.

The calculated upper and lower bound results are shown in Figs. 1 and 2. For the upper bound case, the H atoms produced exhibit multiple velocity groups centered at 11.3, 14.1, 18.4, 30.5, 35.6, 37.2, and 39.8 km/s, see the dotted curve in Fig. 1, while the OH radicals produced can have a velocity group as high as 2.34 km/s, as shown by the dotted curve in Fig. 2. The averaged values of the upper and lower bound velocity distributions of H photofragments are 19.79 and 22.53 km/s, respectively. The corresponding values of the OH radicals are 1.09 and 1.05 km/s, respectively. Our lower bound value is in excellent agreement with that reported by Crovisier [*1989*]. However, the shape of his OH distribution is different from ours. As can be seen from Fig. 2 the calculated shape centered at 1.0 km/s shows high intensity at low OH velocity and gradually decreases toward the high velocity end. The many peaks obtained in the present work may be useful in interpreting the *many peaks* observed in the velocity distributions of the H Ly-α and Hα of comets.

Acknowledgments

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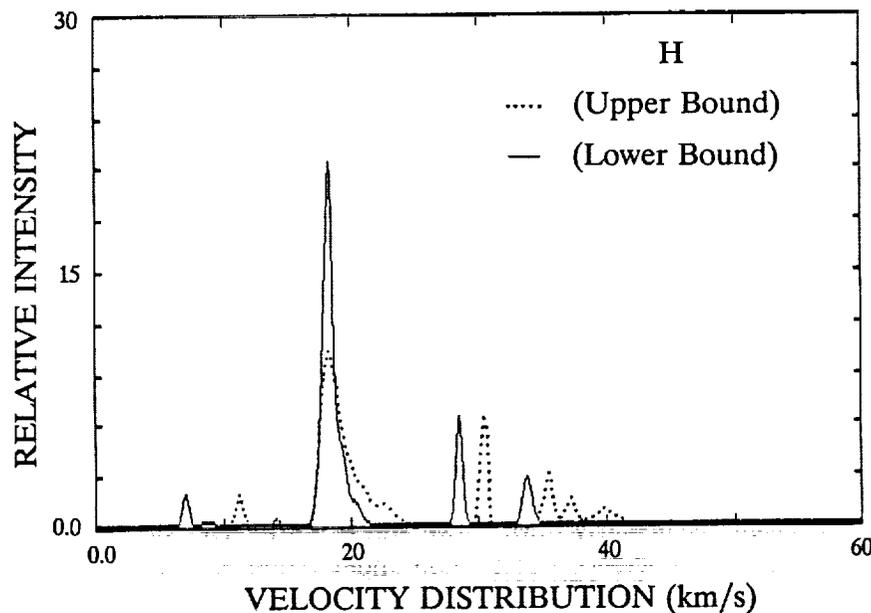

Fig. 1 The velocity distribution of H photofragments produced through solar photodissociation of H_2O. The dashed and solid curves represent the upper and lower bound cases, respectively. See the text for further detail.
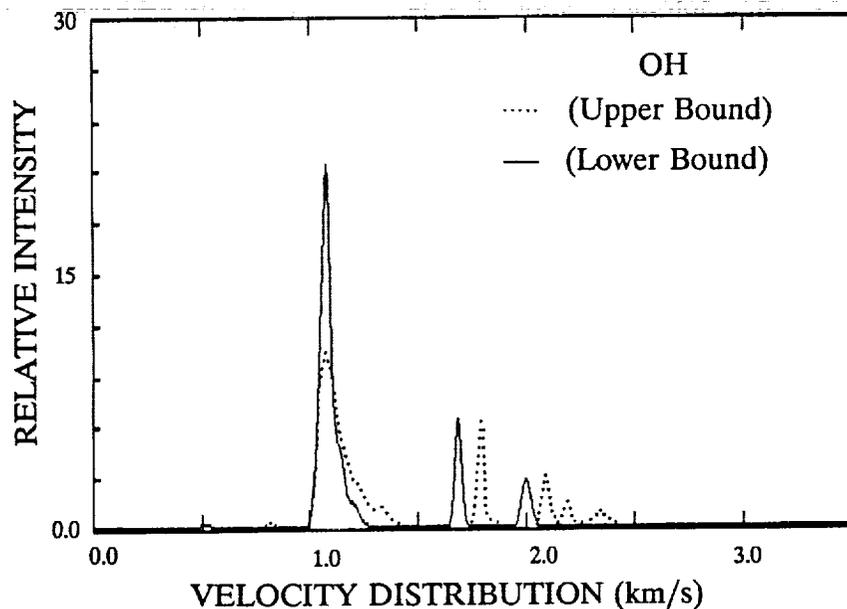

Fig. 2. Same as Fig. 1 except that this is for the velocity distribution of OH photofragments.