A COUPLED CHEMISTRY-EMISSION MODEL FOR ATOMIC OXYGEN GREEN AND RED-DOUBLET EMISSIONS IN THE COMET C/1996 B2 HYAKUTAKE

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ABSTRACT

The green (5577 Å) and red-doublet (6300, 6364 Å) lines are prompt emissions of metastable oxygen atoms in the $1S$ and $1D$ states, respectively, that have been observed in several comets. The value of the intensity ratio of green to red-doublet (G/R ratio) of 0.1 has been used as a benchmark to identify the parent molecule of oxygen lines as H$_2$O. A coupled chemistry-emission model is developed to study the production and loss mechanisms of the O$(1S)$ and O$(1D)$ atoms and the generation of red and green lines in the coma of C/1996 B2 Hyakutake. The G/R ratio depends not only on photochemistry, but also on the projected area observed for cometary coma, which is a function of the dimension of the slit used and the geocentric distance of the comet. Calculations show that the contribution of photodissociation of H$_2$O to the green (red) line emission is 30%–70% (60%–90%), while CO$_2$ and CO are the next potential sources contributing 25%–50% (<5%). The ratio of the photoproduction rate of O$(1S)$ to O$(1D)$ would be around 0.03 (±0.01) if H$_2$O is the main source of oxygen lines, whereas it is ~0.6 if the parent is CO$_2$. Our calculations suggest that the yield of O$(1S)$ production in the photodissociation of H$_2$O cannot be larger than 1%. The model-calculated radial brightness profiles of the red and green lines and G/R ratios are in good agreement with the observations made on the comet Hyakutake in 1996 March.

Key words: comets: general – comets: individual (C/1996 B2 Hyakutake) – molecular processes

1. INTRODUCTION

The spectroscopic emissions from dissociative products in cometary coma are often used in estimating production rates of respective cometary parent species that are sublimating directly from the nucleus (Feldman et al. 2004; Combi et al. 2004). It is a known fact that at smaller (<2 AU) heliocentric distances the inner cometary coma is dominantly composed of H$_2$O. The infrared emissions of H$_2$O molecule are inaccessible from the ground because of strong attenuation by the terrestrial atmosphere. Since H$_2$O does not show any spectroscopic transitions in ultraviolet or visible regions of solar spectrum, one can estimate its abundance indirectly based on the emissions from daughter products, such as OH, O, and H. Thus, tracking emissions of the dissociative products of H$_2$O has become an important diagnostic tool in estimating the production rate as well as in understanding the spatial distribution of H$_2$O in comets (Delsemmme & Combi 1976, 1979; Fink & Johnson 1984; Schulzt et al. 1992; Morgenthaler et al. 2001; Furusho et al. 2006). For estimating the density distribution of H$_2$O from the emissions of daughter species, one has to account for photochemistry and associated emission processes.

The major dissociative channel of H$_2$O is the formation of H and OH, but a small fraction is also possible in O$(^{3}P, ^{1}S, ^{1}D)$ and H$_2$. The radiative decay of metastable $^{1}D$ and $^{1}S$ states of atomic oxygen leads to emissions at wavelengths 6300, 6364 Å (red doublet) and 5577 Å (green line), respectively. The energy levels of atomic oxygen and these forbidden transitions are shown in Figure 1. Even though these emissions are accessible from ground-based observatories, most of the time they are contaminated by telluric night sky emissions as well as emissions from other cometary species. Doppler shift of these lines, which is a function of the relative velocity of comet with respect to the Earth, offers a separation from telluric emissions provided a high-resolution cometary spectrum is obtained. In most of the cometary observations it is very difficult to separate the green line in optical spectrum because of the contamination from cometary C$_2$ (1–2) P-branch band emission. The red line 6300 Å emission is also mildly contaminated by the Q-branch emission of NH$_2$ molecule, but in a high-resolution spectrum this can be easily resolved.

Since these atomic oxygen emissions result due to electronic transitions that are forbidden by selection rules, solar radiation cannot populate these excited states directly from the ground state via resonance fluorescence. The photodissociative excitation and electron impact excitation of neutral species containing atomic oxygen, and ion–electron dissociative recombination of O-bearing ion species, can produce these metastable states (Bhardwaj & Haider 2002). If O$(^{1}D)$ is not quenched by ambient cometary species, then photons at wavelengths 6300 and 6364 Å will be emitted in radiative decay to the ground $^{1}P$ state. Only about 5% of O$(^{1}S)$ atoms result in 2972 and 2958 Å emissions via direct radiative transition to the ground $^{3}P$ state of atomic oxygen. Around 95% of O$(^{1}S)$ decays to the ground state through O$(^{1}D)$ by emitting green line (cf. Figure 1). This implies that if the green line emission is present in cometary coma, the red-doublet emission will also be present, but the opposite is not always true. The average lifetime of O$(^{1}D)$ is relatively small (~110 s) compared to the lifetime of H$_2$O molecule (~8 × 10$^{4}$ s) at 1 AU. The O$(^{1}S)$ also has a very short average lifetime of about 0.1 s. Due to the short lifetime of these metastable species, they cannot travel larger distances in cometary coma before de-exciting via radiative transitions. Hence, these emissions have been used as diagnostic tools to estimate the abundance of H$_2$O in comets (Fink & Johnson 1984; Magee-Sauer et al. 1990; Morgenthaler et al. 2001). The intensity of O[II] emissions, in Rayleigh, can be calculated using the following equation (Festou & Feldman 1981):

$$I = 10^{-6} \tau_{p}^{-1} \alpha \beta N,$$  (1)
where $\tau_p$ is the lifetime of excited species in seconds, $\alpha$ is the yield of photodissociation, $\beta$ is the branching ratio, and $N$ is the column density of cometary species in cm$^{-2}$.

In the case of the red doublet (6300 and 6364 Å), since both emissions arise due to transition from the same excited state ($2P^4 \, 1D$) to the ground triplet state ($2P^4 \, 3P$), the intensity ratio of these two lines should be the same as that of the branching ratio of the corresponding transitions. Using Einstein transition probabilities, Storey & Zeippen (2000) calculated the intensity ratio of the red doublet and suggested that the intensity of 6300 Å would be three times stronger than that of 6364 Å emission, and this has been observed in several comets as well (Spinrad 1982; Fink & Johnson 1984; Morrison et al. 1997; Cochran & Cochran 2001; Capria et al. 2005, 2008; Furusho et al. 2006; Cochran 2008).

The ratio of the intensity of the green line to the sum of intensities of the red doublet can be calculated as

$$\frac{I_{5577}}{I_{6300} + I_{6364}} = \frac{\tau_{green}^1 \alpha_{green} N_{green} \beta_{green}}{\tau_{red}^1 \alpha_{red} N_{red} (\beta_{6300} + \beta_{6364})}. \tag{2}$$

If the emission intensities of the oxygen lines are completely attributed only to photodissociative excitation of H$_2$O and column densities are assumed to be almost the same for both emissions, then the ratio of intensities of the green line to the red doublet is directly proportional to the ratio of $\tau^{-1} \alpha \beta$. Festou & Feldman (1981) reviewed these atomic oxygen emissions in comets. Based on the observation of the O[I] 2972 Å emission in the International Ultraviolet Explorer spectograph of comet Bradfield (1979X), Festou & Feldman (1981) calculated the brightness profiles of red and green emissions. Festou & Feldman (1981) also calculated a theoretical value for the ratio of the intensity of the green line to the red doublet (hereafter referred to as the G/R ratio), which has a value of around 0.1 if H$_2$O is the source for these O[I] emissions in cometary comae, and it is nearly 1 if the source is CO$_2$ or CO. Observations of green and red line emissions in several comets have shown that the G/R ratio is around 0.1, suggesting that H$_2$O is the main source of these O[I] lines. However, since no experimental cross section or yield for the production of O(1S) from H$_2$O is available in the literature, the G/R ratio has been questioned by Huestis & Slanger (2006).

Generally, the red line is more intense than the green line because the production of O(1D) via dissociative excitation of H$_2$O is larger compared to the radiative decay of O(1S). Since the lifetime of O(1D) is larger, quenching is also a significant loss process near the nucleus. So far, the observed G/R ratio in comets is found to vary from 0.022 to 0.3 (Cochran 1984, 2008; Morrison et al. 1997; Zhang et al. 2001; Cochran & Cochran 2001; Furusho et al. 2006; Capria et al. 2005, 2008, 2010).

There are several reactions not involving H$_2$O which can also produce these forbidden oxygen lines (Bhardwaj & Haider 2002). Among the O-bearing species, CO$_2$ and CO also have dissociative channels producing O(1D) and O(1S). However, complex O-bearing molecules (e.g., H$_2$CO, CH$_3$OH, HCOOH) do not produce atomic oxygen as a first dissociative product. Based on the brightness of 6300 Å emission intensity, Delouille & Combi (1976) derived the production rate of O(1D) in comet Bennett 1970 II and suggested that the abundance of CO$_2$ is more than that of H$_2$O. Delouille & Combi (1979) estimated the production of O(1D) in the dissociation of H$_2$O and CO$_2$; about 12% of H$_2$O is dissociated into H$_2$O and O(1D), while 67% of CO$_2$ is dissociated into CO and O(1D). They suggested that a small amount of CO$_2$ can contribute much more than H$_2$O to the red-doublet emission. The model calculations of Bhardwaj & Haider (2002) showed that the production of O(1D) is largely through the photodissociative excitation of H$_2$O, while the major loss mechanism in the innermost coma is quenching by H$_2$O. Cochran & Cochran (2001), based on the observation of the width of the red and green lines, argued that there must be another potential source of atomic oxygen in addition to H$_2$O, which can produce O(1S) and O(1D). Observations of the green and red lines in nine comets showed that the green line is wider than the red line (Cochran 2008), which could be because various parent sources are involved in the production of O(1S).

The model of Glinitskii et al. (2004) showed that the chemistry in the inner coma can produce 1% O$_2$, which can also be a source of red and green lines. Manfroid et al. (2007) also argued, based on light curves, that forbidden O[I] emissions are probably contributed through a dissociation sequence of CO$_2$. A recent observation of comet 17P/Holmes showed that the G/R ratio can be even 0.3, which is the highest reported value so far; suggesting that CO$_2$ and CO abundances might be higher at the time of observation (Capria et al. 2010).

Considering various arguments based on different observations and theoretical works, we have developed a coupled chemistry-emission model to quantify various mechanisms involved in the production of red and green line emissions of atomic oxygen. We have calculated the production and loss rates, and the density profiles, of metastable O(1D) and O(1S) atoms from the O-bearing species, such as H$_2$O, CO$_2$, and CO, and also from the dissociated products OH and O. This model is applied to the comet C/1996 B2 Hyakutake, which was studied through several observations in 1996 March (Biver et al. 1999; Morrison et al. 1997; Cochran & Cochran 2001; Morigenthaler et al. 2001; Combi et al. 2005; Cochran 2008). The line-of-sight-integrated brightness profiles along cometary distances are calculated for 5577 and 6300 Å emissions and compared with the observed profiles of Cochran (2008). We have also evaluated the role of slit dimension, used in the observation, in determining the G/R ratio. The aim of this study is to understand the processes that determine the value of the G/R ratio.
2. MODEL

The neutral parent species considered in this model are H$_2$O, CO$_2$, and CO. We do not consider other significant O-bearing species, such as H$_2$CO and CH$_3$OH, since their first dissociation does not lead to the formation of atomic oxygen atom; the O atom appears in the subsequent photodissociation of daughter products, such as OH, CO, and HCO. On 1996 March 24, the H$_2$O production rate for the comet C/1996 B2 Hyakutake measured by Mumma et al. (1996) was $1.7 \times 10^{29}$ s$^{-1}$. Based on H Ly$\alpha$ emission observation, Combi et al. (1998) measured H$_2$O production rate as $2.6 \times 10^{29}$ s$^{-1}$ on 1996 April 4. Using molecular radio line emissions, Biver et al. (1999) derived the production rates of different species at various heliocentric distances from 1.6 to 0.3 AU. They found that around 1 AU the relative abundance of CO with respect to H$_2$O is high ($\sim 22\%$) in the comet C/1996 B2 Hyakutake.

The number density $n_i(r)$ of the $i$th parent species at a cometocentric distance $r$ in the coma is calculated using the following Haser's formula:

$$n_i(r) = \frac{Q_p}{4\pi v_i r^2} (e^{-\beta_i/r}).$$

Here, $Q_p$ is the total gas production rate of the comet and $v_i$ and $\beta_i$ are the gas expansion velocity (taken as 0.8 km s$^{-1}$; Biver et al. 1999) and the scale length ($\beta_{\text{H}_2\text{O}} = 8.2 \times 10^4$ km, $\beta_{\text{CO}_2} = 5.0 \times 10^5$ km, and $\beta_{\text{CO}} = 1.4 \times 10^6$ km) of the $i$th species, respectively. The Haser model's neutral density distribution has been used in several previous studies for deriving the production rate of H$_2$O in comets based on the intensity of 6300 Å emission (Delsemme & Combi 1976, 1979; Fink & Johnson 1984; Morgenstahler et al. 2001). In our model calculations, the H$_2$O production rate on 1996 March 30 is taken to be $2.2 \times 10^{29}$ s$^{-1}$. The abundance of CO relative to H$_2$O is taken to be 22%. Since there is no report on the observation of CO$_2$ in the comet Hyakutake, we assumed its abundance to be 1% relative to H$_2$O.

However, we vary CO$_2$ abundance to evaluate its effect on the green and red-doublet emissions. The calculations are made when the comet C/1996 B2 Hyakutake was at a heliocentric distance of 0.94 AU and a geocentric distance of 0.19 AU on 1996 March 30. The calculated G/R ratio on other days of the observation is also reported.

The number density of OH produced in the dissociation of parent species H$_2$O at a given cometocentric distance $r$ is calculated using Haser's two-parameter coma model:

$$n_{\text{OH}}(r) = \frac{Q_p}{4\pi v_r r^2} \beta_p (e^{-\beta_r/r} - e^{-\beta_g/r}).$$

Here, $v_r$ is the average velocity of daughter species taken as 1 km s$^{-1}$, and $\beta_p$ and $\beta_g$ are the destruction scale lengths of the parent (H$_2$O, $8.2 \times 10^4$ km) and daughter (OH, $1.32 \times 10^5$ km) species, respectively (Huebner et al. 1992). The solar UV–EUV flux is taken from the SOLAR2000 version 2.3.6 (S2K) model of Tobiska et al. (2000) for the day 1996 March 30, which is shown in Figure 2. For comparison the solar flux used by Huebner et al. (1992) in calculating O(1$D$) and O(1$S$) production rates from various O-bearing species is also presented in the same figure.

The primary photoelectron energy spectrum $Q(E, r, \theta)$ is calculated by degrading solar radiation in the neutral atmosphere using

$$Q(E, r, \theta) = \sum_i \int_\lambda n_i(r) \sigma_i^A(\lambda) I_\infty(\lambda) \exp[-\tau(r, \theta, \lambda)] d\lambda,$$

where

$$\tau(r, \theta, \lambda) = \sum_i \sigma_i^A(\lambda) \sec \theta \int_{r'} n_i(r') dr'.$$

Here, $\sigma_i^A(\lambda)$ and $\sigma_i^I(\lambda)$ are the absorption and ionization cross sections, respectively, of the $i$th species at the wavelength $\lambda$, $n_i(r)$ is its neutral gas density, and $\tau(r, \theta, \lambda)$ is the optical absorption cross section.
depth of the medium at the solar zenith angle $\theta$. $I_{\infty}(\lambda)$ is the unattenuated solar flux at the top of atmosphere at wavelength $\lambda$. All calculations are made at solar zenith angle $\theta$ of $0^\circ$. The total photoabsorption and photoionization cross sections of H$_2$O, CO$_2$, and CO are taken from the compilation of Huebner et al. (1992; http://amop.space.swri.edu), and interpolated at 10 Å bins to make them compatible with the S2K solar flux wavelength bins for use in our model calculations. The total photoabsorption and photoionization cross sections for H$_2$O, CO$_2$, and CO are presented in Figure 3. The photochemical production rates for ionization and excitation of various species are calculated using degraded solar flux and cross sections of corresponding processes (discussed in Section 3) at different cometary distances.

The primary photoelectrons are degraded in cometary coma to calculate the steady state photoelectron flux using the analytical yield spectrum (AYS) approach, which is based on the Monte Carlo method (Singhal & Bhardwaj 1991; Bhardwaj & Singhal 1993; Bhardwaj & Michael 1999a; Bhardwaj & Jain 2009). The AYS method of degrading electrons in the neutral atmosphere can be explained briefly in the following manner. Monoenergetic electrons incident along the $Z$-axis in an infinite medium are degraded in a collision-by-collision manner using the Monte Carlo technique. The energy and position of the primary electron and its secondary or tertiary are recorded at the instant of an inelastic collision. The total number of inelastic events in the spatial and energy bins, after the incident electron and all its secondaries and teritories have been completely degraded, is used to generate numerical yield spectra. These yield spectra contain the yield information about all possible collisional events based on the input electron impact cross sections, resulting in the AYS. This yield spectrum can be used to calculate the steady state photoelectron flux. More details of the AYS approach and the method of photoelectron computation are given in several previous papers (Singhal & Haider 1984; Bhardwaj et al. 1990, 1996; Singhal & Bhardwaj 1991; Bhardwaj 1999, 2003; Bhardwaj & Michael 1999b; Haider & Bhardwaj 2005; Bhardwaj & Jain 2009, 2012; Raghuram & Bhardwaj 2011). The total inelastic electron impact cross sections for H$_2$O are taken from Jackman et al. (1977) and Seng & Linder (1976), and those for CO$_2$ and CO are taken from Jackman et al. (1977). The electron impact cross sections for different dissociative ionization states of H$_2$O are taken from Itikawa & Mason (2005), for CO$_2$ from Bhardwaj & Jain (2009), and for CO from McConkey et al. (2008). The volume excitation rates for different processes are calculated using steady state photoelectron flux and electron impact cross sections. The electron temperature required for ion–electron dissociative recombination reactions is taken from Kőrősmézy et al. (1987). The detailed description of the coupled chemistry-transport model has been given in our earlier papers (Bhardwaj et al. 1995, 1996; Bhardwaj 1999; Bhardwaj & Haider 2002; Haider & Bhardwaj 2005; Bhardwaj & Raghuram 2011). Various reactions involved in the production and loss of metastable O(1S) and O(1D) atoms considered in our model are listed in Tables 1 and 2, respectively.

3. DISSOCIATION OF NEUTRAL SPECIES PRODUCING O(1S) AND O(1D)

3.1. Photodissociation

3.1.1. H$_2$O and OH

The dissociation of H$_2$O molecule starts at wavelengths less than 2424 Å and the primary products are H and OH. But the pre-dissociation process mainly starts from 1860 Å (Watanabe & Zelikoff 1953). The threshold wavelength for the photoionization of H$_2$O is 984 Å. Hence, solar UV photons in the wavelength region 1860–984 Å can dissociate H$_2$O and produce different daughter products. The threshold wavelengths for the dissociation of H$_2$O resulting in the production of O(1S) and O(1D) are 1390 Å and 1770 Å, respectively. Till now, the photoyield value for the production of O(1D) from H$_2$O has been

Figure 3. Total photoabsorption cross sections for H$_2$O, CO$_2$, and CO are shown in the top panel and total photoionization cross sections are shown in the bottom panel. The cross sections are taken from Huebner et al. (1992).
measured in only two experiments. Slanger & Black (1982) measured the $O(1^D)$ yield in the photodissociation of H$_2$O at 1216 Å, and found its value to be 10%. McNesby et al. (1962) reported a 25% yield for the production of $O(1D)$ or $O(3P)$ at 1236 Å from H$_2$O.

Huebner et al. (1992) calculated photoproduction rates for different excited species produced from H$_2$O using absorption and ionization cross sections compiled from different experimental measurements. In our model the cross sections for the production of $O(1D)$ or $O(3P)$ are available. The photorates given by Huebner et al. (1992) are 5.97 $\times$ 10$^{-7}$ s$^{-1}$ and 1.48 $\times$ 10$^{-6}$ s$^{-1}$ for solar quiet and active conditions, respectively. Using the S2K solar EUV–UV flux on 1996 March 30 and cross sections from Huebner et al. (1992; see Figure 4), our calculated value is 8 $\times$ 10$^{-7}$ s$^{-1}$ (cf. Table 2), which is a factor of ~1.5 higher than that of Huebner et al. (1992) for solar minimum condition at 1 AU. This difference in calculated values is mainly due to the higher (a factor of 1.24) value of solar flux at 1216 Å in the S2K model than that used by Huebner et al. (1992; cf. Figure 2).

No experimentally determined cross sections for the production of $O(1S)$ in the photodissociation of H$_2$O are available. The solar flux at H Ly$\alpha$ (cf. Figure 2) is more than an order of magnitude larger than the flux at wavelengths below 1390 Å, which is the threshold for the $O(1S)$ production in the dissociation of H$_2$O. To account for the production of $O(1S)$ in the photodissociation of H$_2$O, we assumed a yield of 0.5% at solar H Ly$\alpha$ (1216 Å). However, to assess the impact of this assumption on the green and red line emissions we varied the yield between 0% and 1%. The calculated photorate for the production of $O(1S)$ from H$_2$O is 6.4 $\times$ 10$^{-8}$ s$^{-1}$ at 1 AU assuming 1% yield at 1216 Å (cf. Table 1).

The primary dissociative product of H$_2$O is OH. The important destruction mechanisms of OH molecule are pre-dissociation through fluorescence process and direct photodissociation. The solar radiation shortward of 928 Å can ionize the OH molecule. The threshold wavelengths for the production of $O(1D)$ and $O(3P)$ in the photodissociation of OH are 1940 and 1300 Å, respectively. The dissociation channels of OH have been discussed by Budzien et al. (1994) and van Dishoeck & Dalgarno (1984). We have used the photorates given by

### Table 1
Reactions for the Production and Loss of $O(1S)$

| Reaction | Rate (cm$^{-3}$ s$^{-1}$ or s$^{-1}$) | Reference |
|----------|-------------------------------------|-----------|
| H$_2$O + h$_v$ $\rightarrow$ O($3S$) + H$_2$ | $6.4 \times 10^{-8}$ | This work |
| OH + h$_v$ $\rightarrow$ O($3S$) + H | $6.7 \times 10^{-8}$ | Huebner et al. (1992) |
| CO$_2$ + h$_v$ $\rightarrow$ O($3S$) + CO | $7.2 \times 10^{-7}$ | This work |
| CO + h$_v$ $\rightarrow$ O($3S$) + C | $4.0 \times 10^{-8}$ | This work |
| H$_2$O + e$_{ph}$ $\rightarrow$ O($3S$) + others | $9.0 \times 10^{-10}$ | This work |
| OH + e$_{ph}$ $\rightarrow$ O($3S$) + others | $2.2 \times 10^{-10}$ | This work |
| CO$_2$ + e$_{ph}$ $\rightarrow$ O($3S$) + others | $4.4 \times 10^{-8}$ | This work |
| CO + e$_{ph}$ $\rightarrow$ O($3S$) + others | $2.2 \times 10^{-10}$ | This work |
| O + e$_{ph}$ $\rightarrow$ O($3S$) | $3.0 \times 10^{-8}$ | This work |
| H$_2$O$^+$ + e$_{ph}$ $\rightarrow$ O($3S$) + others | $4.3 \times 10^{-7}$ | Rosen et al. (2000) |
| OH$^+$ + e$_{ph}$ $\rightarrow$ O($3S$) + others | $6.3 \times 10^{-9}$ | Guberman (1995) |
| CO$_2$ + e$_{ph}$ $\rightarrow$ O($3S$) + others | $2.9 \times 10^{-7}$ | Mitchell (1990) |
| CO + e$_{ph}$ $\rightarrow$ O($3S$) + others | $5.0 \times 10^{-8}$ | Mitchell (1990) |
| O($1S$) + h$_v$ $\rightarrow$ O$^+$ + e | $1.9 \times 10^{-7}$ | Huebner et al. (1992) |
| O($1S$) + e$_{ph}$ $\rightarrow$ O$^+$ + 2e | $2.7 \times 10^{-7}$ | This work |
| O($1S$) $\rightarrow$ O($3P$) + h$_v$2972 | 0.075 | Wiese et al. (1996) |
| O($1S$) $\rightarrow$ O($3D$) + h$_v$5577 | 1.26 | Wiese et al. (1996) |
| O($1S$) + H$_2$O $\rightarrow$ 2OH | $3 \times 10^{-10}$ | Zipf (1969) |
| O($1S$) + CO$_2$ $\rightarrow$ O($3P$) + CO$_2$ | $3 \times 10^{-10}$ $\exp(-1330/T)$ | Atkinson & Welge (1972) |
| O($1S$) + CO $\rightarrow$ O + CO$_2$ | $2.0 \times 10^{-11}$ $\exp(-1327/T)$ | Capetanakis et al. (1993) |
| O($1S$) + CO $\rightarrow$ O$^+$ + CO | $3.21 \times 10^{-12}$ $\exp(-1327/T)$ | Capetanakis et al. (1993) |
| O($1S$) + O$_2$ $\rightarrow$ O$^+$ + CO | $7.4 \times 10^{-14}$ $\exp(-961/T)$ | Capetanakis et al. (1993) |
| O($1S$) + e$_{ph}$ $\rightarrow$ O$^+$ + e | $8.56 \times 10^{-9}$ | Berrington & Burke (1981) |
| O($1S$) $\rightarrow$ O$^+$ + e | $1.56 \times 10^{-9}$ | Berrington & Burke (1981) |
| O($1S$) + O $\rightarrow$ 2O($1D$) | $2.0 \times 10^{-14}$ | Krauss & Neumann (1975) |

**Notes.** The photorates and photoelectron impact rates are at 1 AU on 1996 March 30; $e_{ph}$: photoelectron; $e_{ph}$: thermal electron; $h_v$: solar photon; $T_e$: electron temperature; $T$: neutral temperature.

* This rate is calculated assuming 1% yield for the production of O($1S$) at 1216 Å.
* This work.
* 0.045 is the assumed branching ratio for the formation of O($3S$) via dissociative recombination of H$_2$O$^+$ ion.
* 0.01 is the assumed yield for the formation of O($3D$) via quenching of H$_2$O.
Figure 4. Photodissociative excitation cross sections for the production of O(1D) from H2O, CO2, and CO. These cross sections are taken from Huebner et al. (1992). The "★" represents the cross section value for the production of O(1D) from H2O at 1216 Å assuming 1% yield.

Table 2. Reactions for the Production and Loss of O(1D)

| Reaction | Rate (cm³ s⁻¹ or s⁻¹) | Reference |
|----------|-------------------------|-----------|
| H₂O + hv → O(1D) + H₂ | 8.0 × 10⁻⁷ | This work |
| OH + hv → O(1D) + H | 6.4 × 10⁻⁷ | Huebner et al. (1992) |
| CO₂ + hv → O(1D) + CO | 1.2 × 10⁻⁶ | This work |
| CO + hv → O(1D) + C | 5.1 × 10⁻⁸ | This work |
| O(1S) → O(1D) + hν | 1.26 | Wiese et al. (1996) |
| H₂O + eₚb → O(1D) + H₂ + e | 2.1 × 10⁻¹⁰ | This work |
| OH + eₚb → O(1D) + H + e | 7 × 10⁻¹¹ | This work |
| CO₂ + eₚb → O(1D) + CO + e | 8.5 × 10⁻⁹ | This work |
| CO + eₚb → O(1D) + C(1D) + e | 7 × 10⁻¹¹ | This work |
| O + eₚb → O(1D) | 3.7 × 10⁻⁷ | This work |
| H₂O²⁺ + eₚb → O(1D) + H₂ | 4.3 × 10⁻⁷ (300/Tₑ)⁰.₅ × 0.35⁴ | Rosen et al. (2000) |
| OH + eₚb → O(1D) + H | 6.3 × 10⁻⁷ × (300/Tₑ)⁰.₄⁸ | Guberman (1995) |
| CO₂ + eₚb → O(1D) + CO | 2.9 × 10⁻⁷ (300/Tₑ)⁰.₅ | Mitchell (1990) |
| CO + eₚb → O(1D) + C(1D) | 5 × 10⁻⁸ (300/Tₑ)⁰.₄⁶ | Mitchell (1990) |
| O(1S) + eₚb → O(1D) + e | 1.5 × 10⁻¹⁰ (Tₑ/300)⁰.⁹⁴ | Berrington & Burke (1981) |
| O(S) + H₂O → O(1D) + H₂O | 3 × 10⁻¹⁰ × 0.01ᵇ | Zipf (1969) |
| O(S) + CO₂ → O(1D) + CO₂ | 2.0 × 10⁻¹¹ exp(−1327/T) | Capetanakis et al. (1993) |
| O(S) + CO → O(1D) + CO | 7.4 × 10⁻¹⁴ exp(−961/T) | Capetanakis et al. (1993) |
| O(1D) + hv → O⁺ + e | 1.82 × 10⁻⁷ | Huebner et al. (1992) |
| O(1D) → O(3P) + hν₂₆₃₀₀ | 6.44 × 10⁻³ | Storey & Zeippen (2000) |
| O(1D) → O(3P) + hν₂₆₃₆₄ | 2.15 × 10⁻³ | Storey & Zeippen (2000) |
| O(1D) + eₚb → O⁺ + 2e | 1.75 × 10⁻⁷ | This work |
| O(1D) + eₚb → O(3P) + e | 8.1 × 10⁻¹⁰ (Tₑ/300)⁰.₅ | Link (1982) |
| O(1D) + H₂O → OH + OH | 2.1 × 10⁻¹⁰ | Atkinson et al. (1997) |
| → O(3P) + H₂O | 9.0 × 10⁻¹² | Atkinson et al. (1997) |
| → H₂ + O₂ | 2.2 × 10⁻¹² | Atkinson et al. (1997) |
| O(1D) + CO₂ → O + CO₂ | 7.4 × 10⁻¹¹ exp(−120/T) | Atkinson et al. (1997) |
| → CO + O₂ | 2.0 × 10⁻¹⁰ | Atkinson et al. (1997) |
| O(1D) + CO → O + CO | 5.5 × 10⁻₁⁰ exp(−625/T) | Schmidt et al. (1988) |
| → CO₂ | 8.0 × 10⁻¹¹ | Demore et al. (1997) |

Notes. The photorates and photoelectron impact rates are at 1 AU on 1996 March 30; eₚb: photoelectron; eₚb: thermal electron; hv: solar photon; Tₑ: electron temperature; Tₑ: neutral temperature.

ᵃ 0.35 is the assumed branching ratio for the formation of O(1D) via dissociative recombination of H₂O⁺ ion.
ᵇ 0.01 is the assumed branching ratio for the formation of O(1D) via quenching of H₂O.
Huebner et al. (1992) for the production of O(1D) and O(1S) from an OH molecule whose values are $6.4 \times 10^{-7}$ and $6.7 \times 10^{-8}$ s$^{-1}$, respectively. These rates are based on the dissociation cross sections of van Dishoeck & Dalgarno (1984), which are consistent with the red line observation made by the wide-field spectrometer (Morgenthaler et al. 2007).

3.1.2. CO$_2$

The threshold wavelengths for the dissociation of CO$_2$ molecule producing O(1D) and O(1S) are 1671 Å and 1286 Å, respectively. As noted by Huebner & Carpenter (1979), the rate for this reaction cannot be more than $4 \times 10^{-8}$ s$^{-1}$. We have used this value in our model calculations. This process can be an important source of O(1S) since the comet Hyakutake has a higher CO abundance ($\sim$20%). Using this photorate and CO abundance, we will show that this reaction alone can contribute up to a maximum of 30% to the total O(1S) production.

3.2. Electron Impact Dissociation

In our literature survey we could not find any reported cross section for the production of O(1D) due to the electron impact dissociation of H$_2$O. Jackman et al. (1977) have assembled the experimental and theoretical cross sections for electron impact on important atmospheric gases in a workable analytical form. The cross sections for electron impact on atomic oxygen given by Jackman et al. (1977) have been used to estimate emissions which leave the O atom in the metastable (1D) state. The obtained ratios of 85% in the ground state and 15% in the metastable state are used for the atomic states of C and O produced in the electron impact dissociation of H$_2$O, CO$_2$, and CO. It may be noted that the ground state to metastable state production ratio of 89:11 is observed for atomic carbon and atomic oxygen produced from the photodissociation of CO (Singh et al. 1991). However, as shown later, the contributions of these electron impact processes to the total production of O(1D) are very small (<5%).

Kedzierski et al. (1998) measured the cross section for the electron impact excitation of O(1S) from H$_2$O producing O(1S) with an overall uncertainty of 30%. LeClair & McConkey (1994) measured cross section for the production of O(1S) in the dissociation of CO$_2$ by electron impact; they claimed an uncertainty of 12% in their experimental cross section measurements. The cross section for fragmentation of CO into the metastable O(1S) by electron impact is measured by LeClair et al. (1994). These electron impact cross sections are also recommended by McConkey et al. (2008), and are used in our model for calculating the production rate of O(1S) from H$_2$O, CO$_2$, and CO.

Since the 1D and 1S are metastable states, the direct excitations of atomic oxygen by solar radiation is not an effective excitation mechanism. However the electron impact excitation of atomic oxygen can populate these excited metastable states, which is a major source of airglow emissions in the upper atmospheres of Venus, Earth, and Mars. We calculated the excitation rates for these processes using electron impact cross sections from Jackman et al. (1977). In calculating the photoelectron impact ionization rates of metastable oxygen states, we calculated the cross sections by changing the threshold energy parameter for ionization of neutral atomic oxygen in the analytical expression given by Jackman et al. (1977). The above-mentioned electron impact cross sections for the production of O(1S) from H$_2$O, CO$_2$, CO, and O, used in the current model, are presented in Figure 5 along with the calculated photoelectron flux energy spectrum at a cometocentric distance of 1000 km.

3.3. Dissociative Recombination

The total dissociative recombination rate for H$_2$O$^+$ reported by Rosen et al. (2000) is $4.3 \times 10^{-7}$ cm$^{-3}$ s$^{-1}$ at 300 K. The channels of dissociative recombination have also been studied by this group. It was found that the dissociation process is...
dominated by three-body breakup (H + H + O) that occurs with a branching ratio of 0.71, while the fraction of two-body breakup (O + H₂) is 0.09, and the branching ratio for the formation of OH + H is 0.2. The maximum kinetic energy of the dissociative products forming atomic oxygen produced in ground state is 3.1 eV and 7.6 eV for the three- and two-body dissociation, respectively. Since the excitation energy required for the formation of metastable O(1S) is 4.19 eV, the three-body dissociation cannot produce oxygen atoms in the 1S state. However, the O(1D) atom can be produced in both, the three-body and the two-body, breakup dissociation processes. To incorporate the contribution of H₂O⁺ dissociative recombination in the production of O(1D) and O(1S), we assumed that 50% of branching fraction of the total recombination in three-body and two-body breakups lead to the formation of O(1D) and O(1S) atoms, respectively. For dissociative recombination of CO₂⁺, CO⁺, and OH⁺ ions, we assumed that the recombination rates are the same for the production of both O(1D) and O(1S). We will show that these assumptions affect the calculated O(1S) and O(1D) densities only at larger (≥10⁴ km) cometocentric distances, but not in the inner coma. Tables 1 and 2 list the rates, along with the source reference, for these recombination reactions.

4. RESULTS AND DISCUSSION

4.1. Production and Loss of O(1S) Atom

The calculated O(1S) production rate profiles for different processes in the comet C/1996 B2 Hyakutake are presented in Figure 6. These calculations are made under the assumption...
of 0.5% yield of O(1S) from H₂O at 1216 Å solar H Lyα line and 1% CO₂ relative abundance. The major production source of O(1S) is the photodissociative excitation of H₂O throughout the cometary coma. However, very close to the nucleus, the photodissociative excitation of CO₂ is also an equally important process for the O(1S) production. Above 100 km, the photodissociative excitation of CO₂ and CO makes an equal contribution in the production of O(1S). Since the cross section for the electron impact dissociative excitation of H₂O, CO₂, and CO is small (see Figure 5), the contributions from electron impact dissociation to O(1S) production are smaller by an order of magnitude or more than that due to photodissociative excitation. At larger cometocentric distances (>2 × 10³ km), the dissociative recombination of H₂O⁺ ion is a significant production mechanism for O(1S), whose contribution is higher than those from the photodissociative excitation of CO₂ and CO. The dissociative recombination of other ions do not make any significant contribution to the production of O(1S).

In the inner coma, the calculated production rates of O(1S) via photodissociative excitation is CO₂ at various wavelengths are presented in Figure 7. The major production of O(1S) occurs in the wavelength region 955–1165 Å where the average cross section is ≈2 × 10⁻¹⁷ cm² (cf. Figure 4) and the average solar flux is ≈1 × 10⁹ photons cm⁻² s⁻¹ (cf. Figure 2). The calculated loss rate profiles of O(1S) for major processes are presented in Figure 8. Close to the nucleus (<50 km), quenching by H₂O is the main loss mechanism for metastable O(1S). Above 100 km, the radiative decay of O(1S) becomes the dominant
loss process. The contributions from other loss processes are orders of magnitude smaller and hence are not shown in Figure 8.

4.2. Production and Loss of O(1D) Atom

The production rates as a function of cometocentric distance for various excitation mechanisms of the O(1D) are shown in Figure 9. The major source of O(1D) production in the inner coma is the photodissociation of H$_2$O. The wavelength-dependent production rates of O(1D) from H$_2$O are presented in Figure 10. The O(1D) production in the photodissociation of H$_2$O is governed by solar radiation at H Ly$\alpha$ (1216 Å) wavelength. However, very close to the nucleus, the production of O(1D) is largely due to photons in the wavelength region 1165–1375 Å. Since the average absorption cross section of H$_2$O decreases in this wavelength region by an order of magnitude, the optical depth at wavelengths greater than 1165 Å is quite small (see Figure 3). Hence, these photons are able to travel deeper into the coma unattenuated, thereby reaching close to the nucleus where they dissociate H$_2$O producing O(1D). Thus, at the surface of the comet, the production of O(1D) is controlled by the solar radiation in this wavelength band.

In high production rate comets, the production of O(1D) near the nucleus would be governed by solar photons in this wavelength region. The production of O(1D) from H$_2$O by solar photons from other wavelength regions is smaller by more than an order of magnitude.

After the photodissociative excitation of H$_2$O, the next significant O(1D) production process at radial distances below 50 km is the photodissociative excitation of CO$_2$. Above 50 km to about 1000 km, the radiative decay of O(1S) and at radial...
distances above 1000 km the dissociative recombination of H$_2$O$^+$ are the next potential sources of the O(1D) (see Figure 9). The calculated wavelength-dependent production rates of O(1D) for the photodissociation of CO$_2$ are shown in Figure 11. Solar radiation in the wavelength region 1165–955 Å dominates the O(1D) production. Since the cross section for the production of O(1D) due to the photodissociation of CO$_2$ is more than an order of magnitude higher in this wavelength region compared to the cross section at other wavelengths (see Figure 4), the solar radiation in this wavelength band mainly controls the formation of O(1D) from CO$_2$. Other potential contributions are made by solar photons in the wavelength band 1585–1375 Å at distances <50 km, and 955–745 Å at radial distances >100 km. Since the CO$_2$ absorption cross section around 1216 Å is smaller by more than two orders of magnitude compared to its maximum value, the solar radiation at H Ly$\alpha$ is not an efficient source of O(1D) atoms.

Zipf (1969) measured the total rate coefficient for the quenching of O(1S) by H$_2$O as $3 \times 10^{-10}$ cm$^3$ s$^{-1}$. The primary channel in quenching mechanism is the production of two OH atoms. The production of O(1D) is also a possible channel whose rate coefficient is not reported in the literature. Hence, we assumed that 1% of the total rate coefficient can lead to the formation of O(1D) in this quenching mechanism. However, this assumption has no implications on the O(1D) production since the total contribution due to O(1S) is about three orders of magnitude smaller than the major production process of O(1D).

The calculated loss rate profiles of O(1D) are presented in Figure 12. Below 1000 km, the O(1D) can be quenched by
various cometary species. The quenching by H$_2$O is the major loss mechanism for O($^1D$) below 500 km. Above 2 $\times$ 10$^3$ km radiative decay is the dominant loss process for O($^1D$).

4.3. Calculation of Green and Red-doublet Emission Intensity

Using the calculated production and loss rates due to various processes mentioned above, and assuming photochemical equilibrium, we computed the number density of O($^1S$) and O($^1D$) metastable atoms. The calculated number densities are presented in Figure 13. The O($^1D$) density profile shows a broad peak around 200–600 km. But, in the case of O($^1S$), the density peaks at much lower radial distances of $\sim$60 km. The number densities of O($^1D$) and O($^1S$) are converted into emission rate profiles for the red-doublet and green line emissions, respectively, by multiplying with Einstein transition probabilities as

$$V_{(6300+6364)}(r) = A_{(6300+6364)} \times [O^1D(r)]$$

$$= A_{(6300+6364)} \frac{\sum_{i=1}^{k} P_i(r)}{\sum_{i=1}^{k} L_i(r) + A^{(1)}D}$$

(7)

and

$$V_{(5577)}(r) = A_{(5577)} \times [O^1S(r)] = A_{(5577)} \frac{\sum_{i=1}^{k} P_i(r)}{\sum_{i=1}^{k} L_i(r) + A^{(1)}S}$$

(8)

where \([O^1S(r)]\) and \([O^1D(r)]\) are the calculated number density for the corresponding production rates \(P_i(r)\) and loss frequencies \(L_i(r)\) for O($^1S$) and O($^1D$), respectively. \(A^{(1)}D\) and \(A^{(1)}S\) are the total Einstein spontaneous emission coefficients for red-doublet and green line emissions. Using the emission rate profiles, the line-of-sight intensity of green and red-doublet emissions along the projected distance \(z\) is calculated as

$$I(z) = 2 \int_{z}^{R} V_{(5577, 6300+6364)}(s) ds,$$

(9)

where \(s\) is the abscissa along the line of sight and \(V_{(5577, 6300+6364)}(s)\) is the emission rate for the green or red-doublet emission. The maximum limit of integration \(R\) is taken as 10$^5$ km. The calculated brightness profiles of 5577 and 6300 Å emissions are presented in Figure 14. These brightness profiles are then averaged over the projected area corresponding to the slit dimension 1$''$2 $\times$ 8$''$2 centered on the nucleus of the comet C/1996 B2 Hyakutake for the observation on 1986 March 30 (Cochran 2008). The G/R ratio averaged over the slit is also calculated.

4.4. Model Results

Morrison et al. (1997) observed the green and red-doublet emissions on the comet C/1996 B2 Hyakutake in the high-resolution optical spectra obtained on 1996 March 23 and 27 and found the G/R ratio in the range 0.12–0.16. Cochran (2008) observed the 5577 and 6300 Å line emissions on this comet on 1996 March 9 and 30, with the G/R ratio as 0.09 for March 9 observation. We calculated the G/R ratio by varying the yield for O($^1S$) production in the photodissociation of H$_2$O at 1216 Å (henceforth referred to as the O($^1S$) yield). Since CO$_2$ is not observed in this comet, we assumed that a minimum of 1% CO$_2$ is present in the coma. However, we also carried out calculations for 0%, 3%, and 5% CO$_2$ abundances in the comet. We calculated the contributions of different production processes in the formation of O($^1S$) and O($^1D$) at three different projected distances of 10$^3$, 10$^4$, and 10$^5$ km from the nucleus for the above-mentioned CO$_2$ abundances and the O($^1S$) yield values varying from 0% to 1%. These calculations are presented in Table 3. The percentage contribution of major production processes in the projected field of view for the green and red-doublet emissions is also calculated. The G/R ratio is calculated after averaging the intensity over the projected area 165 $\times$ 1129 km, which corresponds to the dimension of the slit used in the observation made by Cochran (2008) on 1996 March 30. These calculated values are presented in Table 4.

Taking 1% CO$_2$ abundance and 0% O($^1S$) yield, the calculated percentage contributions of major production processes of the O($^1S$) and O($^1D$) atoms are presented in Table 3. Around 60%–90% of the O($^1D$) is produced from the photodissociation of H$_2$O. Contributions of the photodissociative excitation of CO$_2$
and CO in the production of O(1S) and O(1D) are 15%–40% and 1%, respectively. Around 10^4 km projected distance, the photodissociative excitation of OH (∼20%) and the dissociative recombination of H_2O^+ (∼30%) are also significant production processes for the O(1S) atoms. However, the contributions from these processes in O(1D) production is only around 10%.

For CO_2 abundance of 1% and O(1S) yield of 0.2%, the calculations presented in Table 3 show that the photodissociation of H_2O contributes around 20%–40% in the production of O(1S) and 60%–90% in the production of O(1D) atom. The next major source of O(1S) production is the photodissociation of CO_2 and CO with each contributing ∼10%–25%. The relative contributions from the photodissociation of parent species H_2O, CO_2, and CO to O(1S) and O(1D) production decreases with an increase in projected distance from the nucleus. At 10^4 km projected distance, the photodissociation of OH contributes 15% and 8% to the production of O(1S) and O(1D) atoms, respectively. Above 1000 km projected distance, the contribution of H_2O^+ dissociative recombination to O(1S) production is around 20%. The production of the O(1D) atom is mainly via the photodissociation of H_2O, but around 10^4 km the dissociative recombination of H_2O^+ ion is also a significant production process contributing around 12%. At 10^4 km, the dissociative recombination of OH^+ ion is also a significant production process contributing around 12%. At 10^4 km the dissociative recombination of H_2O^+ ion is also a significant production process contributing around 12%. At 10^4 km, the dissociative recombination of OH^+ also contributes around 10% to the total O(1D) production, which is not shown in Table 3, and this value is independent of the O(1S) yield or CO_2 abundance.

Table 3

| O(1S) | Production Processes of O(1S) and O(1D) at Three Cometocentric Projected Distances (km) |
|-------|--------------------------------------------------------------------------------------------|
| Yield | hν + H_2O | hν + OH | hν + CO_2 | e + H_2O^+ | O(1S) → O(1D) | hν + CO |
| (%)   | 10^2     | 10^3   | 10^4     | 10^2  | 10^3   | 10^4 |

Notes. Calculations are made for 1996 March 30, when r = 0.94 AU and Δ = 0.19 AU.

b Yield for the production of O(1S) from the photodissociation of H_2O at solar Lyα (1216 Å) line.

b The values in square brackets are for the O(1S) yield.
Radiative decay of O(1S) is a minor (<5%) production process in the formation of O(1D).

We also calculated the relative contributions of different processes in the formation of green and red line emissions in the slit projected field of view, which are presented in Table 4. For the above case, the photodissociation of H2O contributes around 35%, while the photodissociation of CO2 and CO contributes 23% and 22%, respectively, to the production of green line emission. The contribution of dissociative recombination of H2O+ ions is around 10%. The major production process of red lines is the photodissociation of H2O (90%); the dissociative recombination of H2O+ and radiative decay of the O(1S) atom are minor (<5%) production processes. With the O(1S) yield of 0.2% and 1% CO2 abundance, the slit-averaged G/R ratio is found to be 0.11.

When the O(1S) yield is increased to 0.5% with 1% CO2 abundance (see Table 3), the contribution from the photodissociative excitation of H2O to the O(1S) production is increased, with values varying from 35% to 60%, while the contribution to O(1D) production is not changed. In this case, the contribution from the photodissociation of CO2 and CO to the O(1S) production is reduced (values between 10% and 15%). The contributions from other processes are not changed significantly. Table 4 shows that in this case of around 60% of green line in the slit projected field of view is produced via the photodissociation of H2O, while the contributions from the photodissociation of CO2 and CO are around 15% each. The main (90%) production of red-doublet emission is through the photodissociation of H2O. The slit-averaged G/R ratio is 0.17.

On further increasing the O(1S) yield to 1% with CO2 abundances of 1%, the contribution of photodissociation of H2O to O(1S) atom production is further increased (values between 50% and 75%), while the contribution from photodissociation of CO2 and CO is decreased to around 10% each (cf. Table 3). The contributions from other processes are not affected compared to the previous case. As seen from Table 4, in this case the contribution of photodissociation of H2O to green line is around 75% in the slit projected field of view, while contributions from the photodissociation of CO2 and CO are decreased to 10% each. The calculated G/R ratio is 0.27 (Table 4).

We also evaluated the effect of CO2 on the red-doublet and green line emissions by varying its abundance to 0%, 3%, and 5%. The calculated percentage contribution of major processes along the projected distances and in the slit projected field of view are presented in Tables 3 and 4, respectively. In the absence of CO2, the contributions from H2O, H2O+, and CO in O(1S) production are increased by ~10% (cf. Tables 3 and 4). Taking 0% O(1S) yield and by increasing CO2 relative abundance from 1% to 3%, the percentage contributions for O(1S) from the photodissociative excitation of CO2 (CO) are increased (decreased) by 50%. The contribution from H2O to O(1D) production is not changed.

The calculations presented in Tables 3 and 4 depict that the contributions of various processes are significant in the production of O(1S) atom, whereas the photodissociative excitation of H2O is the main production process for the O(1D) atom. Since the comet C/1996 B2 Hyakutake is rich in CO (abundance ~22%) compared to other comets, the contribution from CO photodissociation to O(1S) production is significant (10%–25%). In the case of a comet having CO abundance less than 20%, the major production source of the metastable O(1S) atom would be the photodissociation of H2O and CO2.

### 4.5. Comparison with Observations

In 1996 March, the green and red-doublet emissions were observed in the comet C/1996 B2 Hyakutake from two ground-based observatories (Morrison et al. 1997; Cochran 2008). Each observatory determined the G/R ratio using a different slit size. Using a circular slit, the projected radial distance over the comet for the Morrison et al. (1997) observation on March 23 and 27 varied from 640 to 653 km, while for the Cochran (2008) observation, using a rectangular slit, the projected area was 480 × 3720 km on March 9 and 165 × 1129 km on March 30. The clear detection of both green and red-doublet emissions and determination of the G/R ratio could be done for March 9 and 23 observations only (Cochran 2008; Morrison et al. 1997).

### Table 4

Calculated Percentage Contribution for the Major Production Processes of the Green (Red-doublet) Emission in the Slit Projected Field of View on the Comet C/1996 B2 Hyakutake

| O(1S) Yield (%) | hv + H2O | hv + OH | hv + CO2 | e− + H2O⁺ | O(1S) → O(1D) | hv + CO | G/R Ratiob |
|-----------------|----------|---------|----------|-----------|---------------|---------|-----------|
| 1% CO2          | 0.0      | 0 [91]  | 2 [0.5]  | 36 [1]    | 13 [3]        | 1 [1]   | 35 [1]    | 0.07      |
|                 | 0.2      | 36 [91] | 1 [0.5]  | 23 [1]    | 8 [3]         | 3 [3]   | 22 [1]    | 0.11      |
|                 | 0.5      | 59 [89] | 1 [0.5]  | 14 [1]    | 5 [3]         | 4 [4]   | 14 [1]    | 0.17      |
|                 | 1.0      | 76 [87] | 0.5 [0.5]| 10 [1]    | 0.5 [3]       | 6 [6]   | 10 [1]    | 0.27      |
| 0.0 CO2         | 0.0      | 0 [94]  | 4 [0.5]  | 0 [0]     | 21 [3]        | 1 [1]   | 59 [1]    | 0.04      |
|                 | 0.2      | 49 [93] | 2 [0.5]  | 0 [0]     | 11 [3]        | 2 [2]   | 30 [1]    | 0.08      |
|                 | 0.5      | 70 [91] | 1 [0.5]  | 0 [0]     | 6 [3]         | 4 [4]   | 17 [1]    | 0.15      |
|                 | 1.0      | 82 [89] | 0.5 [0.5]| 0 [0]     | 3 [3]         | 6 [6]   | 10 [1]    | 0.25      |
| 3% CO2          | 0.0      | 0 [87]  | 1 [0.5]  | 60 [4]    | 7 [3]         | 3 [3]   | 20 [1]    | 0.13      |
|                 | 0.5      | 35 [82] | 0.5 [0.5]| 45 [6]    | 3 [3]         | 7 [7]   | 7 [1]     | 0.27      |

**Notes.**

*a* The values in square brackets are the calculated percentage contribution for the red-doublet emission.

*b* The calculated values are averaged over the projected area of 165 × 1130 km corresponding to the slit size of 1′′ × 8′′ at Δ = 0.19 AU centered on the nucleus of the comet C/1996 B2 Hyakutake on 1996 March 30 (Cochran 2008).
observed G/R ratio was 0.09 and 0.12–0.16 for the observation on March 9 and 23, respectively.

Performing a very high resolution ($R = 200,000$) observation of the comet C/1996 B2 Hyakutake on 1996 March 30, Cochran (2008) obtained radial profiles of 5577 and 6300 Å lines. In Figure 14, we have compared the model-calculated intensity profiles of 6300 and 5577 Å lines at different projected cometocentric distances with the observation of Cochran (2008). The calculated G/R ratio along the projected distance is shown in Figure 15. The 6300 Å emission shows a flat profile up to $\sim 500$ km, whereas the 5577 Å green line starts falling off beyond 100 km. This is due to the quenching of O($3S$) and O($3D$) by H$_2$O in the innermost coma (cf. Figures 8 and 12), thereby making both the production and loss mechanisms controlled by H$_2$O. Above these distances, the emissions are mainly controlled by the radiative decay of $3S$ and $3D$ states of oxygen atoms.

Similar to the calculations presented in Tables 3 and 4, in Figures 14 and 15 we present the red and green line intensity profiles and the G/R ratios, respectively, for different contributions of O($3S$) yield and CO$_2$ abundances. Since the photodissociative excitation of H$_2$O is the main production process for the O($3D$) atom, the red line intensity is almost independent of the variation in O($3S$) yield and CO$_2$ abundance. In the case of 0% CO$_2$ abundance, the best fit to the observed green line profile is obtained when the O($3S$) yield is $\sim 0.5\%$ ($\pm 0.1\%$), where the G/R ratio varies from 0.06 to 0.26 (cf. Figure 15) and the slit-averaged G/R ratio for March 30 observation is 0.15 (cf. Table 4). The shape of green line profile cannot be explained with 1% or 0% O($3S$) yield, while the case for 0.2% O($3S$) yield can be considered as somewhat consistent with the observation. For this case, the value of G/R ratio shown in Figure 15 is found to vary over a large range from 0.54 to 0.02.

When we consider 1% CO$_2$ in the comet, the best-fit green profile is obtained when the O($3S$) yield is $\sim 0.2\%$. The case for 0.5% O($3S$) yield also provides the green line profile consistent with the observation. In both these cases the G/R ratio varies between 0.32 and 0.04 over the cometocentric projected distances of 10 to $10^4$ km. The calculated 5577 Å profiles for the O($3S$) yield of 0% and 1% are inconsistent with the observed profile.

In Figure 14 we also show a calculated profile for a case when the CO$_2$ abundance is 3% while the O($3S$) yield is 0% (i.e., no O($3S$) is produced in the photodissociation of H$_2$O). The calculated 5577 Å green line profile shows a good fit to the observed profile: suggesting that even a small abundance of CO$_2$ is enough to produce the required O($3S$). This is because the CO$_2$ is about an order of magnitude more efficient in producing the O($3S$) atom than H$_2$O in the photodissociation process (see Table 1). However, since O($3S$) would definitely be produced in the photodissociation of H$_2$O, and that the CO$_2$ would surely be

![Figure 15](image.png)

**Figure 15.** Calculated green to red-doublet intensity ratio along projected distances for different CO$_2$ relative abundance [CO$_2$] and yield [Yld] for O($3S$) production in the photodissociation of H$_2$O. G/R is the calculated green to red-doublet intensity ratio averaged over the slit projected size 165 × $1130$ km for C/1996 B2 Hyakutake on 1996 March 30.

| Yield | 0.1 | 0.2 | 0.5 | 1   | 1.5 | 2   |
|-------|-----|-----|-----|-----|-----|-----|
| 1% CO$_2$ |     |     |     |     |     |     |
| 0.0   | 0.11| 0.07| 0.05| 0.04| 0.04| 0.04|
| 0.2   | 0.17| 0.11| 0.07| 0.06| 0.05| 0.05|
| 0.5   | 0.26| 0.17| 0.10| 0.08| 0.07| 0.07|
| 1.0   | 0.40| 0.26| 0.15| 0.12| 0.10| 0.10|
| 0% CO$_2$ |     |     |     |     |     |     |
| 0.0   | 0.07| 0.05| 0.03| 0.03| 0.03| 0.03|
| 0.2   | 0.13| 0.09| 0.05| 0.05| 0.04| 0.04|
| 0.5   | 0.23| 0.15| 0.09| 0.07| 0.06| 0.06|
| 1.0   | 0.37| 0.24| 0.14| 0.11| 0.01| 0.01|
| 3% CO$_2$ |     |     |     |     |     |     |
| 0.0   | 0.19| 0.13| 0.08| 0.06| 0.06| 0.06|
| 0.5   | 0.33| 0.21| 0.13| 0.10| 0.09| 0.09|

**Notes.** Calculations are made for 1996 March 30, where $r = 0.94$ AU.

*O($3S$) yield from the photodissociation of H$_2$O.*
present in the comet (though in smaller abundance), the most consistent value for the O(1S) yield would be around 0.5%. Assuming 5% CO2 and 0.5% O(1S) yield, the calculated green line emission profile is inconsistent with the observation (cf. Figure 15). In this case, the calculated G/R ratio shown in Figure 15 is found to vary between 0.24 and 0.05.

From the above calculations, it is clear that the slit projected area on to the comet also plays an important role in deciding the G/R ratio. This point can be better understood from Table 5 where the G/R ratio is presented for a projected square slit on the comet at different geocentric distances. It is clear from this table that for a given physical condition of a comet and a given heliocentric distance, the observed G/R ratio for a given slit size can vary according to the geocentric distance of the comet. For example, for an O(1S) yield of 0.2% (0.5%) and CO2 abundance of 1%, the G/R ratio can be 0.17 (0.26) if the comet is very close to the Earth (0.1 AU), whereas the G/R ratio can be 0.07 (0.1), 0.06 (0.08), or 0.06 (0.07), if the comet, at the time of observation, is at a larger distance of 0.5, 1, and 2 AU from the Earth, respectively. Furthermore, a G/R ratio of ~0.1 can be obtained even for the O(1S) yield of 0%. This suggests that the value of 0.1 for the G/R ratio is in no way a definitive benchmark value to conclude that H2O is the parent of atomic oxygen atom in the comet, since smaller (~5% relative to H2O) amounts of CO2 and CO itself can produce enough O(1S) compared to that from H2O. This table also shows that for observations made around a geocentric distance of 1 AU, the G/R ratio would be generally closer to 0.1. The G/R ratio observed in different comets ranges from 0.02 to 0.3 (e.g., Cochran 2008; Capria et al. 2010).

Thus, we can conclude that the G/R ratio not only depends on the production and loss mechanisms of the O(1S) atom, but also depends on the nucleocentric slit projected area over the comet. Moreover, the CO2 plays an important role in the production of O(1S), and thus the green line emission, in comets. With the present model calculations and based on the literature survey of dissociation channels of H2O, we suggest that the O(1S) yield from the photodissociation of H2O cannot be more than 1% of the total absorption cross section of H2O at solar Lyα radiation. The best-fit value of the O(1S) yield derived from Figure 14 for a smaller (1%) CO2 abundance in the comet C/1996 B2 Hyakutake is 0.4% (±0.1)%. As per Tables 1 and 2, this means that the ratio of rates of O(1S) to O(1D) production in the H2O photodissociation should be 0.03 (±0.01), which is much smaller than the value of 0.1 generally used in the literature based on Festou & Feldman (1981). Furthermore, if the source of red and green lines is CO2 (CO), the ratio of photorates for O(1S) to O(1D) would be around 0.6 (0.8) (see Tables 1 and 2).

To verify whether the O(1S) yield of 0.5% (for the CO2 abundance of 1%) derived from Figure 14, based on the comparison between model and observed red and green line radial profiles in the comet Hyakutake on 1996 March 30, is consistent with the G/R ratio observed on other days on this comet, we present in Table 6 the G/R ratio calculated for observations made on 1996 March 9, 23, 27, and 30, along with the observed value of G/R ratio from Morrison et al. (1997) and Cochran (2008). These calculations are made by taking the solar flux on the day of observation using the Tobiska (2004) SOLAR2000 model and scaled according to the heliocentric distance of the comet on that date. The CO abundance is 22%, the same as in all the calculations presented in the paper.

The calculated G/R ratio on March 9, when the geocentric distance was 0.55 AU and the H2O production rate was 5 × 10^28 s^-1, is 0.09 (see Table 6) which is the same as the observed ratio obtained by Cochran (2008). On March 23 and 27, the comet is closer to both the Sun and Earth (geocentric distance ~0.1 AU) and its H2O production rate was four times higher than the value on March 9. The calculated G/R ratio on March 23 is 0.12, which is in agreement with the observed ratio obtained by Morrison et al. (1997).

### 5. CONCLUSIONS

The green and red-doublet atomic oxygen emissions are observed in the comet C/1996 B2 Hyakutake in 1996 March when it was passing quite close to the Earth (Δ = 0.1–0.55 AU). A coupled chemistry-emission model has been developed to study the production of green (5577 Å) and red-doublet (6300 and 6364 Å) emissions in comets. This model has been applied to the comet Hyakutake and the results are compared with the observed radial profiles of 5577 and 6300 Å line emissions and the green to red-doublet intensity ratio. The important results from the present model calculations can be summarized as follows. It may be noted that some of these results enumerated below may vary for other comets having different gas production rate or heliocentric distance.

1. The photodissociation of H2O is the dominant production process for the formation of O(1D) throughout the inner cometary coma. The solar H Lyα (1216 Å) flux mainly governs the production of O(1D) in the photodissociative emission of atomic oxygen in comets.
3. The collisional quenching of $O(1^D)$ atoms by H$_2$O is significant up to a radial distance of ~1000 km; above this distance, the radiative decay is the main loss mechanism of $O(1^D)$ atoms. The collisional quenching of $O(1^D)$ by other neutral species is an order of magnitude smaller.

4. The photodissociation of H$_2$O is the major process for the production of O(1S) atoms, but near the nucleus the photodissociation of CO$_2$ can be the dominant source. The solar H Ly$\alpha$ (1216 Å) flux controls the production of O(1S) via photodissociative excitation of H$_2$O.

5. At cometocentric distances of <100 km, the main loss processes of O(1S) is quenching by H$_2$O molecule, while above 100 km the radiative decay is the dominant loss process.

6. Since the photoabsorption cross section of the CO$_2$ molecule is quite small at 1216 Å, the contribution of CO$_2$ in the production of O(1S) and O(1D) at the solar H Ly$\alpha$ is insignificant.

7. Because the CO$_2$ absorption cross section in the 1165–955 Å wavelength range is higher by an order of magnitude compared to that at other wavelengths, the solar radiation in this wavelength region mainly controls the production of O(1D) and O(1S) in the photodissociative excitation of CO$_2$. Moreover, the CO$_2$ absorption cross section in this band is also the largest compared to those of H$_2$O and CO.

8. The cross section for the photodissociation of H$_2$O producing O(1S) at the solar H Ly$\alpha$ wavelength (with 1% O(1S) yield) is smaller by more than two orders of magnitude than the cross section for the photodissociation of CO$_2$ producing O(1S) in the wavelength region 1165–955 Å. Though the solar flux at 1216 Å is higher compared to that in the 1165–955 Å wavelength region by two orders of magnitude, the larger value of the CO$_2$ cross section in this wavelength band enables CO$_2$ to be an important source for the production of metastable O(1S) atom.

9. In the case of CO, the dissociation and ionization thresholds are close to each other. Hence, most of the solar radiation ionizes the CO molecule rather than producing the O(1S) and O(1D) atoms.

10. Though the CO abundance is relatively high (~22%) in the comet C/1996 B2 Hyakutake, the contribution of CO photodissociation in the O(1D) production is small (~1%), while for the production of O(1S) its contribution is 10%–25%.

11. The photoelectron impact dissociative excitation of H$_2$O, CO$_2$, and CO makes only a minor contribution (<1%) in the formation of metastable O(1S) and O(1D) atoms in the inner coma.

12. The O(1S) density peaks at shorter radial distances than the O(1D) density. The peak value of O(1S) density is found around 60 km from the nucleus, while for the O(1D) a broad peak around 200–600 km is observed.

13. In an H$_2$O-dominated comet, the green line emission is mainly generated in the photodissociative excitation of H$_2$O with a contribution of 40%–60% (varying according to the radial distance) to the total intensity, while the photodissociation of CO$_2$ is the next potential source contributing 10%–40%.

14. For the red line emission the major source is the photodissociative excitation of H$_2$O, with contribution varying from 60% to 90% depending on the radial distance from the nucleus.

15. The G/R ratio depends not only on the production and loss processes of the O(1S) and O(1D) atoms, but also on the size of observing slit and the geocentric distance of comet at the time of observation.

16. For a fixed slit size, the calculated value of the G/R ratio is found to vary between 0.03 and 0.5 depending on the geocentric distance of the comet. In the innermost (<300 km) part of the coma, the G/R ratio is always larger than 0.1, with values as high as 0.5. On the other hand, at cometocentric distances larger than 1000 km the G/R ratio is always less than 0.1.

17. The model-calculated radial profiles of 6300 and 5577 Å lines are consistent with the observed profiles on the comet C/1996 B2 Hyakutake for the O(1S) yield of 0.4 (±0.1) and CO$_2$ abundances of 1%.

18. The model-calculated G/R ratio on the comet Hyakutake is in good agreement with the G/R ratio observed on two days in 1996 March by two observatories using different slit sizes.

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