AN S$_2$ FLUORESCENCE MODEL FOR INTERPRETING HIGH-RESOLUTION COMETARY SPECTRA. I. MODEL DESCRIPTION AND INITIAL RESULTS

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ABSTRACT

A new versatile model providing S$_2$ fluorescence spectrum as a function of time is developed with the aim of interpreting high-resolution cometary spectra. For the S$_2$ molecule, it is important to take into account both chemical and dynamic processes because S$_2$ has a short lifetime and is confined in the inner coma, where these processes are most important. The combination of the fluorescence model with a global coma model allows for the comparison with observations of column densities taken through an aperture and for the analysis of S$_2$ fluorescence in different parts of the coma. Moreover, the model includes the rotational structure of the molecule. Such a model is needed for interpreting recent high spectral resolution observations of cometary S$_2$. A systematic study of the vibrational-rotational spectrum of S$_2$ is undertaken, including relevant effects, such as nonequilibrium state superposition and the number density profile within the coma due to dynamics and chemistry, to investigate the importance of the above effects on the scale length and abundance of S$_2$ in comets.

Subject headings: comets: general — molecular processes — ultraviolet: solar system

1. INTRODUCTION

Although comets hold important clues to the formation of the solar system, there is no complete picture of where comets formed (Mumma al. 2000; Irvine et al. 2000). The mixing ratio of the minor constituents of frozen gases in the ice-dust conglomerate of the nucleus is a very important clue to the original composition of the frozen gases in the solar nebula, but it is not well understood. A detailed and comprehensive description of production of minor species, such as S$_2$, and their sources, and the inner coma chemistry are prerequisites for unambiguous characterization of the nucleus. Understanding comets, in turn, yields insights into the origin of the solar system.

Several sulfur species have been detected in comets, including S$_2$, which has a short lifetime and is concentrated in the innermost coma. The proximity of comet IRAS-Araki-Alcock 1983d (A’Hearn, Feldman, & Schleicher 1983a) and comet Hyakutake C/1996 B2 (Weaver et al. 1996; Laffont et al. 1998) to Earth favored the detection of emission lines of such a short-lived species. Recently, S$_2$ has been detected in comet Lee C/1999 H1 (Feldman et al. 1999).

Up to now, pure vibrational models were used to analyze these data. Kim, A’Hearn, & Larson (1990), using a multicycle fluorescence model, derived an abundance of 2.5$x10^{-4}$ relative to water in International Ultraviolet Explorer (IUE) spectra of comet IRAS-Araki-Alcock. The model developed by Laffont et al. (1998) shows that there is a fast evolution of S$_2$ fluorescence spectra in proportion to the age of the molecule as it undergoes the solar radiation and consequently to its distance from the nucleus. On the basis of this model, it was possible to set an upper limit to the abundance of 10$^{-4}$ relative to water from IUE observations of comet Hyakutake, which is consistent with the abundance derived from HST observations a few days later (Weaver et al. 1996; A’Hearn et al. 1999). The abundance of S$_2$ in comet Lee is (3–5) $x10^{-5}$ relative to water (Feldman et al. 1999).

After a time-dependent model of the vibrational population of S$_2$ was applied to the fullest extent, it appeared that a more extensive model including the rovibrational structure of S$_2$ was needed to provide additional clues about the physical and chemical nature of the inner coma of comets, especially since high spectral and spatial resolution cometary spectra containing S$_2$ exist now. In this paper, we describe such a model suitable for interpreting high-resolution spectra of S$_2$. We combine the resulting spectra with a global coma model based on gas dynamics and chemistry. This is important for cometary applications and makes it possible to follow the time evolution of S$_2$ fluorescence in the inner coma.

Section 2.1 describes the model and presents our method of calculation. Synthetic S$_2$ spectra at various ages of the molecule are presented in § 3.1. In § 3.2, we compare this model with the pure vibrational model and point out important consequences of using a pure vibrational model for analyzing spectra of even moderate resolution. We apply our model to such observations, the IUE spectra of comet IRAS-Araki-Alcock in which S$_2$ was first detected and discuss the effects on the abundance and lifetime determinations. In § 3.3, we explore the possible applications of this model for cometary observations, with both high spatial and spectral resolution. Finally, we summarize our conclusions and give directions for future model enhancements in § 4.

2. MODEL DESCRIPTION

2.1. Time-Dependent Fluorescence Model

The B $^3\Sigma_u^+ - X^3\Sigma_g^+$ system of S$_2$ has been analyzed in detail in the laboratory (see, e.g., Ikenoue 1960; Heaven,
Coma Chemistry Model

We have developed a global model for the reactive multi-fluid gas flow in the coma, including gas release from the nucleus, the relationship of chemical abundances in the coma to those in the nucleus ices (depending on heliocentric distance of the comet), entrainment of dust by escaping coma gases, and fragmentation and evaporation of dust (distributed coma sources) (Huebner et al. 1991; Boice, Benkhoff, & Gladstone 1995). The model solves the fluid dynamic equations for the mass, momentum, and energy of three neutral fluids (atomic and molecular hydrogen and the heavier bulk fluid) and the electrons. In the inner coma, the gas expands, cools, accelerates, and undergoes a plethora of photolytic (with optical depth effects) and gas-phase chemical reactions that transform the dozen or so parent molecules into hundreds of daughter species. Beyond the collision region, the multifluid gas flow for fast atomic hydrogen, fast molecular hydrogen, electrons, and the bulk of the coma gas undergoes a transition from fluid dynamic flow to free molecular flow.
The model produces cometocentric abundances of the coma gas species, velocities of the bulk gas, light atomic and molecular hydrogen with escape, and electrons, gas and electron temperatures, column densities to facilitate comparison with observations, coma energy budget quantities, attenuation of the solar irradiance, and other quantities that can be related readily to observations. Model results are integrated in the line of sight for direct comparison with observations.

Several mechanisms have been proposed to explain the presence of S$_2$ in the coma of comets (Vanysek 1993; Saxena & Misra 1995; A’Hearn et al. 2000). For our initial model we assume the simplest possible case: direct release of S$_2$ from the nucleus with a production rate of $10^{-4}$ that of water, in order to simulate observations of comet Hyakutake (Laffont et al. 1998; A’Hearn et al. 1999). The S$_2$ molecule photodissociates at one of three assumed rates: 100 s (Meier et al. 1999), 200 s (de Almeida & Singh 1986; Budzien & Feldman 1992), and 450 s (A’Hearn et al. 1983a), as this rate is not well known. No dust was included for this work. With such simple chemistry, we have used our coma model to incorporate dynamical and optical depth effects accurately, since S$_2$ is confined to the innermost region of the coma, where these effects are most important.

3. RESULTS

3.1. Synthetic Fluorescence Spectra

Individual synthetic fluorescence spectra of S$_2$ are presented in Figure 1 as a function of age of the molecule,
obtained considering an irradiation equivalent to the solar irradiation at a heliocentric distance of 1 AU. At short times, corresponding to small cometocentric distances, the brightest lines are in the range 280–300 nm (e.g., the 9–0 band at 282.9 nm and the 7–1 band at 296.1 nm) and the intensity of these lines does not change a lot with age \( t \). These lines correspond to transitions from the levels \( v_0 = 7 \) to 9 that reach a value close to the steady state value within 1 s, as shown on Figure 2a. This figure represents the population of the vibrational levels in the \( B \)-state, which is the sum of the population of the rotational levels in one vibrational level. When the time increases, the lower vibrational levels are populated and the lines at long wavelengths become brighter, such as the 3–3 band at 324.5 nm or the 2–3 band at 328.9 nm.

After roughly 100 s, the relative intensities of the lines are nearly constant (see Fig. 1). But inside a vibrational level, the population of the higher rotational levels continue to slowly increase, approaching steady state with the solar irradiation, to the detriment of the lower rotational levels.

### 3.2. Comparison with the Pure Vibrational Model

Our pure vibrational, time-dependent model tended to show that the fluorescence spectrum varies the most between \( t = 0 \) and 200 s, when the intensities have reached 90% of the steady-state values, but very little afterward until about 600 s, when steady state is effectively achieved (Fig. 2b). This result is different from the one deduced from our rovibrational model which shows that the global population of the vibrational levels are constant after about 100 s. The numerous rotational levels allow the electrons to reach higher levels at a faster rate due to the overestimate of the Einstein coefficients for the emission when ignoring the rotational levels.

Using a pure vibrational model to interpret the relative intensities can lead to errors in estimating the effective solar irradiation time of \( S_2 \) in the coma which can affect its derived lifetime against destructive processes. Indeed, the \( S_2 \) lifetime is not a well known parameter. The lifetime deduced from observations in comet IRAS-Araki-Alcock (A'Hearn et al. 1983a; Budzien 

### 3.3. Application to Cometary \( S_2 \)

#### 3.3.1. \( S_2 \) Fluorescence in a Column of the Coma

An observation of a given region of the coma gives the superposition of emissions of all the molecules in a column. These molecules are at different cometocentric distances, they have different age \( t \), and hence have undergone different solar irradiation times. In order to model the \( S_2 \) cometary fluorescence, we combined our fluorescence model with a global coma model based on dynamics and chemistry as described in § 2.2 (Huebner et al. 1991; Boice et al. 1995; Boice & Benkhoff 1996). The number density \( n \) of \( S_2 \) given by the coma model is shown in Figure 3 as a function of age \( t \) and distance to the nucleus surface \( R \) for different lifetimes: \( \tau = 100, 200, \) and 450 s.
bands of maximum intensity are indicated in both cases.

chemistry for three values of the lifetime: the distance to the nucleus given by the model based on gas dynamics and to the nucleus. We observe a shift in intensity from the 7–1 band, whereas at 73 km from the nucleus, the maximum of emissions has shifted to the 2–3 band. Also, bands at longer wavelengths are stronger relative to the brightest bands.

Up to now, we considered an initial temperature of 200 K, which is a correct assumption if S₂ is released from the nucleus. Other mechanisms for the formation of S₂ have been proposed, involving chemical reactions (Saxena & Misra 1995; A'Hearn et al. 2000) or a grain source (Vanysek 1993). For these alternative assumptions, the excitation of S₂ when it is formed is different. However, if we consider an initial temperature of 400 K, the effects due to the initial distribution are not perceptible when integrating over the line of sight as soon as one observes a few kilometers away from the nucleus.

Practically, we do not observe only one column in the coma but many within an aperture A, for instance a slit or a hole:

$$F_{\lambda}(t, \rho) = \int_{-\pi/2}^{\pi/2} F_{\lambda}(t, \rho, \theta) \frac{\rho}{\cos^2 \theta} d\theta,$$

where $F(t)$ is the synthetic spectrum obtained at the time $t$ since formation of the molecule, $n(t)$ is the number density at the distance $R$ from the nucleus surface reached by the molecule in $t$, and $\rho$ is the projected distance of the column to the nucleus surface. The angle $\theta$ varies from $-\pi/2$ to $\pi/2$ to include the whole column. We have ignored the Greenstein effect for molecules within the column.

The superimposed nonequilibrium spectra that would be detected on the surface of the nucleus and 73 km away from it are plotted in Figure 4, using a lifetime of 200 s. The number density decreases by more than $10^3$ from the nucleus to 73 km away, which causes an important decrease in the emission intensity. Moreover, we observe a shift in intensity from the $\approx 280$–300 nm region to the $\approx 330$–380 nm region. The maximum of emissions on the nucleus is the 7–1 band, whereas at 73 km from the nucleus, the maximum of emissions has shifted to the 2–3 band. Also, bands at longer wavelengths are stronger relative to the brightest bands.

Fig. 3.—Number density of S₂ molecules vs. the age of the molecule and the distance to the nucleus given by the model based on gas dynamics and chemistry for three values of the lifetime: $\tau = 100$, 200, and 450 s.

We weighted the individual fluorescence spectra with the number density given by the coma model as follows:

$$F_{\lambda}(t, \rho) = \int_{-\pi/2}^{\pi/2} F_{\lambda}(t, \rho, \theta) \frac{\rho}{\cos^2 \theta} d\theta,$$

where $F(t)$ is the synthetic spectrum obtained at the time $t$ since formation of the molecule, $n(t)$ is the number density at the distance $R$ from the nucleus surface reached by the molecule in $t$, and $\rho$ is the projected distance of the column to the nucleus surface. The angle $\theta$ varies from $-\pi/2$ to $\pi/2$ to include the whole column. We have ignored the Greenstein effect for molecules within the column.

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It is important to integrate the weighted spectra within an aperture for simulating real observations. The spectrum will be different depending on the width of the slit, or if the slit is centered or off-centered from the nucleus. For instance, we can simulate an observation with a slit having an aperture of $0^\circ 87 \times 7''$ or $68 \times 580 \text{ km}^2$ centered on the nucleus. This case actually simulates ground-based observations of comet Hyakutake by Meier et al. (1999). The simulated spectra are shown in Figure 5 for the lifetimes $\tau = 450$, 200, and 100 s. Considering a short lifetime leads to a smaller intensity, but the shape of the spectrum is also different depending on $\tau$ (in particular, the relative intensities between the 280–310 nm region and the rest of the spectrum vary considerably). This fact is not relevant for spectra such as IUE spectra where the maximum wavelength is about 320 nm but it may be interesting to consider in the case of visible spectra such as the ones obtained by Meier et al. (1999). We also considered the effect of having the same slit off-centered with an offset of $2''$. A'Hearn et al. (1999) reported that with such an offset, S₂ was no longer detected. With $\tau = 450 \text{ s}$, the intensities are reduced by a factor of $\approx 3$ compared to observations with a slit centered on the nucleus. This factor is 5 with $\tau = 200 \text{ s}$ and 12 with $\tau = 100 \text{ s}$.

Fig. 4.—Simulation of the fluorescence emission of S₂ molecules within a column very close to the surface nucleus and 73 km away from the nucleus. The bands of maximum intensity are indicated in both cases.
3.3.2. $S_2$ Fluorescence at High Spectral Resolution

Another application of this model is the interpretation of high spectral resolution spectra. Figure 6 shows the synthetic rotational structure of the 1–5 band for a molecule of age $t = 200$ s. This band is superimposed with the faint 6–8 band (dotted line). Also shown are the modeled lines convolved with a FWHM Gaussian of 0.2 Å that corresponds to ground-based observations of comet Hyakutake (Meier et al. 1999). The left-hand scale is related to the line intensity before convolution. The right-hand scale gives the $g$-factor, or fluorescence efficiency, of the lines.

![Figure 6: Synthetic rotational structure of the 1–5 band (solid line) superimposed on the faint 6–8 band (dotted line) for a 200 s solar irradiation time at 1 AU from the Sun. The lines are convolved with a FWHM Gaussian of 0.2 Å that corresponds to ground-based observations of comet Hyakutake (Meier et al. 1999). The left-hand scale is related to the line intensity before convolution. The right-hand scale gives the $g$-factor, or fluorescence efficiency, of the lines.](image)

The upper spectrum in Figure 7 is obtained for a molecule with an age of 1 s. The two bands, 7–4 and 9–6, are dominant. The intensity of these bands, particularly the 7–4 band, decreases relative to the other bands when the exposure time increases. The dominance of these bands in a

they are contaminated by stronger emission lines such as bands of OH (0–0), OH (1–1), and NH (0–0). Due to no constraint on temperature, the rotational temperature given by the modeled spectrum is too high compared to the 45 K observed rotational temperature (Kim 2000).

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table}

### Table 1: Most Intense Bands Predicted by the Model after a Solar Irradiation of 200 s

| Band  $v_B - v_X$ | $\lambda_{\text{origin}}$ (nm) | Relative Intensity |
|----------|-----------------|-----------------|
| 1–5     | 349.9           | 1.00            |
| 2–4     | 336.7           | 0.98            |
| 2–3     | 328.9           | 0.97            |
| 1–4     | 341.6           | 0.90            |
| 3–3     | 324.5           | 0.72            |
| 1–6     | 358.6           | 0.69            |
| 3–4     | 332.1           | 0.66            |
| 2–5     | 344.8           | 0.64            |
| 4–2     | 313.1           | 0.62            |
| 3–2     | 317.2           | 0.61            |
| 0–6     | 364.2           | 0.61            |
| 1–3     | 333.6           | 0.57            |
| 5–2     | 309.2           | 0.53            |

**Notes.** $\lambda_{\text{origin}}$ is the wavelength of the band origin. The relative intensity is integrated within the band once the lines are convolved with a 0.2 Å FWHM Gaussian corresponding to observations of comet Hyakutake from Kitt Peak Observatory (Meier et al. 1999). $^a$ Bands detected in comet Hyakutake (Meier et al. 1999). $^b$ Overlapping with NH (0–0). $^c$ Overlapping with OH (1–1). $^d$ Overlapping with OH (0–0).
spectrum with high spatial resolution is therefore a strong indication of freshly released S$_2$ molecules.

4. CONCLUSION

We developed a time-dependent fluorescence model of S$_2$ and combined it with a global coma model, for interpreting observations in different coma regions. As it takes into account the rotational structure of the molecule, it can also be used to analyze high spectral resolution observations, such as those obtained in comet Hyakutake. We point out that it is also important to consider the rotational levels of S$_2$ in the fluorescence calculations to interpret even moderate-resolution spectra such as IUE spectra. We also demonstrated the need of a time-dependent model to allow better estimates of the lifetime and to determine the lines characteristic of the freshly released molecules.

In this work, we concentrated on linking the physics and chemistry of the coma and the cometary fluorescence. This is the first time to our knowledge that a gas dynamics model with chemistry has been coupled with a time-dependent fluorescence model to analyze cometary emissions, representing a leap forward in our ability to gain insight into the physical and chemical processes in the inner coma and the nature of parent species. This global model with many detailed processes in the inner coma has great potential to resolve issues regarding the detailed rotational lines intensities as functions of distance from the nucleus, collision frequency, and production rates and to gain insights into the composition into the cometary nucleus. To this end, the future direction of this work will be to investigate coma temperature profiles, the effects due to optical depth in the inner coma for the emergent S$_2$ emissions, and also the role of collisions. Considering collisions would allow self-consistent calculations of the rotational temperature for direct comparison to observations. Using the global coma model, we will also consider a more complete chemistry of S$_2$, not only photolysis for the production and destruction of S$_2$ in cometary comae.

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Fig. 7.—Evolution with age of the molecule of the S$_2$ bands at 1 AU from the Sun. The theoretical lines are convolved with a 0.2 Å FWHM Gaussian. The two bright bands in the upper graph are characteristic of newly released S$_2$. The bands detected in comet Hyakutake (Meier et al. 1999) are indicated in the lower graph. The model shows that these bands are already predominant after 45 s of solar irradiation. The bands in parentheses may also have been detected but were weaker. Bands contaminated by stronger cometary emissions, such as OH and NH, are indicated.
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Note added in proof. — Recently, S₂ was identified in the spectra of comet Ikeya-Zhang C/2002 C1 obtained with the STIS instrument of HST (H. A. Weaver et al., BAAS, 34, 12.04 [2002]). At first glance, our model is consistent with the observed spectra.