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POSSIBLE EMISSION STRUCTURE OF C_2H IN THE 2.5 MICRON INFRARED SPECTRA OF COMETS

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ABSTRACT

We have constructed a synthetic spectrum of the 2.5 micron C_2H bands and compared them with diminutive structures in the near-infrared spectra of Comets P/Halley and West (1976 VI). We found that the Q branches of the C_2H bands coincide with two small emission peaks in the spectra of the comets. We undertook Monte Carlo simulations using observed emission intensities of C_2 and possibly C_2H in Comet P/Halley in order to derive a lifetime range of C_2H and a production rate at the time of observations of P/Halley. We obtained a C_2H production rate of $1 \times 10^{27} sec^{-1}$ for P/Halley on December 20, 1985, assuming the 2.5 micron features are due to C_2H. We derived a very short lifetime (<100 seconds) of C_2H at 1 AU heliocentric distance, assuming that the only parent molecule for C_2H and C_2 is C_2H_2. Using this short lifetime we were unable to fit our C_2 distribution model to C_2 distribution curves observed by O'Dell et al.(1988), because our curve shows a steep slope compared with the observed one. We conclude that there must be significant additional source(s) for C_2H and C_2 other than C_2H_2.

Keywords : control of telescope, driving of telescope, tracking efficiency pointing accuracy

1. INTRODUCTION

The C_2 bands are the most prominent emission in the visible region of cometary spectra along with other strong molecular emissions, such as NH_2 and CN bands. However, the parent molecule(s) of C_2 have not been unambiguously identified thus far. The number of parent molecules has been proposed including C_2H_2, C_3, C_2H_4, CHON particles, etc. Jackson et al.(1991) proposed that reaction chains, $C_2H_2 + h\nu \rightarrow C_2 + H_2$ and $C_2H_2 + h\nu \rightarrow C_2H + H + h\nu \rightarrow C_2 + H + H$, should be the major chemistry to create C_2 in cometary comae, and the branching ratios of the above reaction should be 21 and 79%, respectively. O'Dell et al. (1988) claimed that C_2 should be the third generation analyzing the C_2 distribution curves of Comet P/Halley, which showed a flat slope between 250 and 6300 km from the nucleus. Recently, there have been investigations on diffuse source of C_2 in Comet Hyakutake (Laffont et al. 1998) and Comet P/Halley (Rousselot et al. 1994). Rousselot et al. proposed that there should be two different origins for the C_2 molecules: a main one in the nucleus, and a secondary one in a dust jet of CHON grains. Therefore, it is important to identify possible intermediate molecules, such as C_2H, and its lifetime against solar ultraviolet lights in order to confirm/disconfirm whether the $C_2H_2 \rightarrow C_2H \rightarrow C_2$ chain is the major reaction.

Although C_2H has not been detected in cometary infrared spectra, it has two strong electronic bands at 2.5 microns. In this paper, we study the 2.5 micron C_2H bands spectroscopically, and construct a synthetic spectrum. We present comparisons between the model and the observed infrared spectra of Comets P/Halley and West (1976 VI). Recent bright comets, such as Comets Hale-Bopp and Hyakutake, could not provide better infrared spectra to reveal the 2.5 micron C_2H spectral structures (Private communications with Dr. H. Campins, 1998). In the spectra of Comets P/Halley and West, we find two small emission peaks, which approximately coincide with the Q branch positions of the two C_2H bands. Using the emission intensities, available lifetimes of C_2H_2, C_2H, and C_2 in the literature, and observation parameters, we perform Monte Carlo simulations. We present production rates of C_2H_2, C_2H, and C_2 for Comet P/Halley. We derive a range of the lifetimes of C_2H, assuming that the parent molecule

of C_2H and C_2 is C_2H_2. Using the obtained lifetime range, we construct a C_2 distribution curve and compare it with the observed C_2 curves of O'Dell et al. (1988) to test whether the $C_2H_2 - C_2H - C_2$ chain is an important chemical reaction.

2. OBSERVATIONS

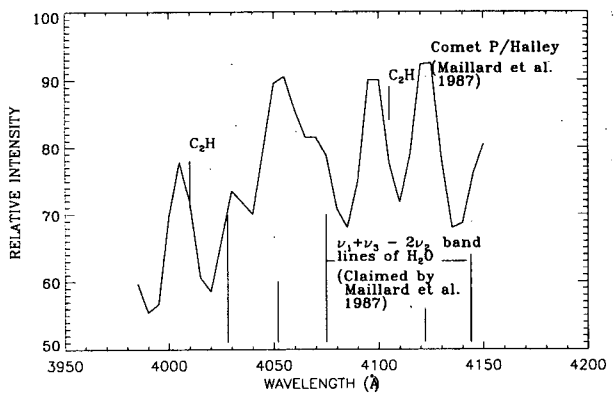

Figure 1a.— see Figure 1b

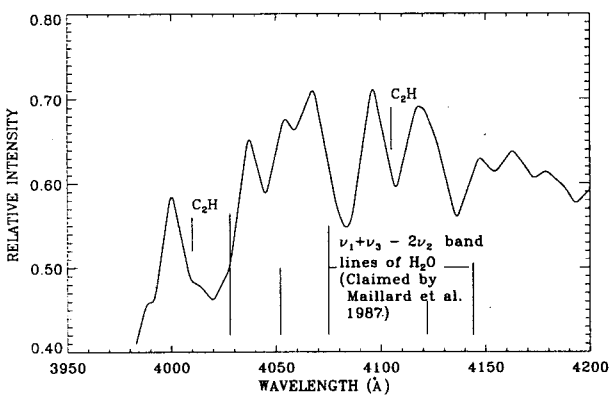

Figure 1b.— Figures 1a and 1b. Original Comets P/Halley (1a) and West (1b) spectra observed by Maillard et al. (1987) and Johnson et al. (1983), respectively. The positions of the C_2H bands and H_2O lines, are marked. The H_2O lines are tentatively claimed by Maillard et al.

Detailed descriptions for the observations of Comets P/Halley and West were presented by Maillard et al. (1987) and Johnson et al. (1983), respectively. The two observations were made by Fourier Transform Spectrometers. In Figures 1a and 1b, the observed spectra are shown for the 3950 – 4200 cm^{-1} range of Comets P/Halley and West, respectively. As seen in the figures, the positions of the Q branches of C_2H, and H_2O lines are marked. The H_2O lines were tentatively claimed by Maillard et al. based on Figure 1a.

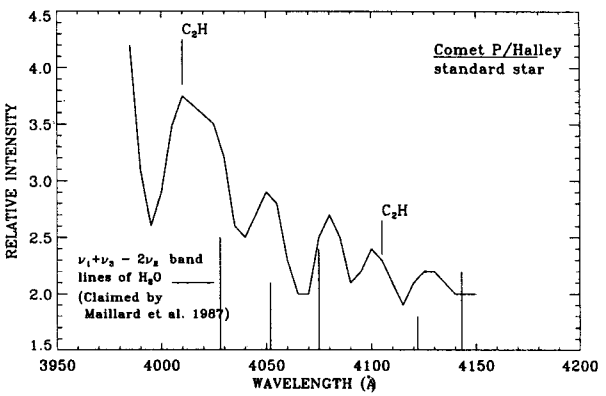

Figure 2a.— see Figure 2b

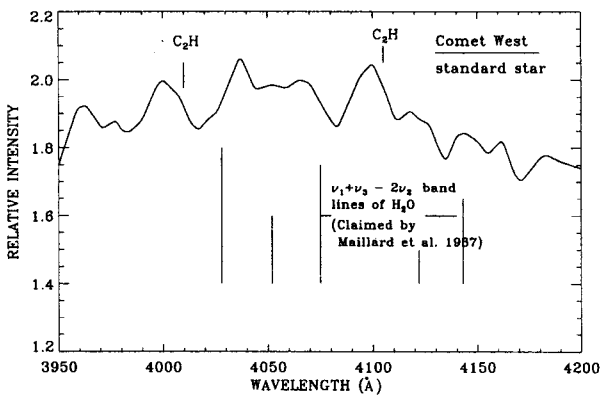

Figure 2b.— Figures 2a and 2b. Ratioed spectra of Comets P/Halley (1a) and West (1b) using standard stars, respectively (see the main text for detailed explanations). The C_2H band emissions become dominant structures, whereas they are positioned only on the shoulders of the strong peaks in Figs. 1a and 1b.

Figures 2a and 2b present ratioed spectra, which were obtained by dividing the spectra in Figures 1a and 1b by standard star spectra. We ratioed the comet spectra with the standard star spectra (i.e., comet spectra ÷ standard star spectra) instead of using a subtraction (i.e., comet spectra – standard star spectra) in order to reveal the molecular emission lines. The reason is the following: In this spectral range, the thermal emission of dust particles strongly influences the continuum and therefore it is difficult to determine an exact continuum level to reveal weak emission lines by subtracting the strong continuum. As seen in the P/Halley spectrum in Figure 2a, the emission peaks at 4010 and 4103

cm^{-1} coincide with the C_2H band positions, which are only on the shoulders of the observed peaks in Figure 1a. Also shown in the West spectrum in Figure 2b, it is clear that the C_2H peaks become dominant features, whereas in Figure 1b they are only minor features on the shoulder of the observed peaks. It is also noted that the comparisons between the H_2O lines and other emission peaks in the $4000 - 4100\ cm^{-1}$ range are much better in the ratioed spectra in Figures 2a and 2b than in Figures 1a and 1b. Maillard et al. (1987) derived an intensity of $1.7 \times 10^{-7} Wm^{-2}sr^{-1}$ for the entire emission feature, which includes the suspected H_2O lines. Based on the above analysis, we estimate the emission intensity of the C_2H bands to be approximately $2 \times 10^{-8} Wm^{-2}sr^{-1}$.

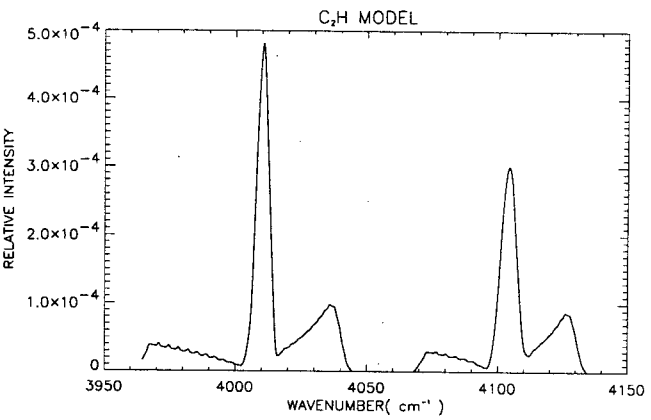

Figure 3.— A model spectrum of the C_2H bands, which have been convolved with the same instrument function used for the observations of Comet West.

3. MODELLINGS

3.1. 2.5 Micron C_2H Band Models

The $A^2\Pi - X^2\Sigma$ electronic band system of C_2H occurs between 1 to 3 micron range. The line positions of this system were measured and documented by Curl, Carrick, and Merer (1985). A fluorescence lifetime of the bands at 2.5 micron, which is greater than 60 microseconds, was measured by Shokoohi et al. (1986). Using the lifetime, the Einstein A coefficient of the bands is estimated to be approximately $1.0 \times 10^4 sec^{-1}$, which is at least 1000 times of that of a typical ro-vibrational infrared band. In order to calculate the fluorescence efficiency factors (g-factors) of the bands, solar radiation intensities are required for the spectral range. According to high resolution spectra obtained from the ATMOS (Atmospheric Trace Molecule Spectroscopy) instrument on the Spacelab 3 mission in 1983 (Farmer and Norton, 1989), the solar spectra in the $4005 - 4015$ and $4100 - 4110\ cm^{-1}$ ranges show only sporadic weak absorption lines and their absorptions are less than 20% of the solar continuum. Therefore we do not expect significant Swings effects in the spectral ranges. In this paper, therefore, we use a low resolution solar spectrum compiled by Arvesen et al. (1969) for the calculation of a g-factor for simplifying the calculations. For individual line intensities, we adopted Franck-Condon formulae for the $^2\Pi - {}^2\Sigma$ transitions presented by Earls (1935). Since the Einstein A coefficients of other bands in the A–X system are not well known, we did not attempt a complete fluorescence calculation including all the rotational transitions in the A–X bands to derive the g-factor. The estimated g-factor for the bands at 4010 and 4103 cm^{-1} is about $3.5 \times 10^{-2} sec^{-1} molecule^{-1}$, and the resultant model spectrum is presented in Figure 3.

3.2. Monte Carlo Simulations

Monte Carlo simulations were carried out assuming an isotropic outflow of a parent(C_2H_2) molecule from the nucleus. The decaying products of parent and daughter species are assumed to be moving in random directions in the reference frames of parents or daughters. The velocities of the decaying products are based on estimated or known excess energies of photodissociations of the precursor molecules. The maximum possible velocity occurs when all the excess energy is transferred to the kinetic energy of the decaying product. The simulations were carried out for both two and three generation decay processes. Although the Monte Carlo code is capable of using time-varying parent production rates, as we will discuss later, we assumed a steady-state parent production rate. This means that we are essentially modelling steady-state two- and three-generation vectorial models. If there are more than one reaction involved, the corresponding branching ratios were used to arrive at the final result. See Table 1 for the details of the photodissociation reactions of C_2H_2, C_2H and C_2, precursor lifetimes, and the velocities of decaying products.

It is noted that the higher accuracy of derived results can be obtained, if both C_2H and C_2 observations were made closer in time. However, in the absence of such data for Comet P/Halley, we used observations of C_2H and C_2 made in close proximity in time – The C_2H

Table 1. Input parameters for the Monte Carlo simulations. Notice that we used extreme values for a conservative calculation.

Photodissociation reaction	Precursor lifetime(sec) at 1 AU	Maximum decay product velocity(km/sec)
$C_2H_2 + h\nu \rightarrow C_2H + H$	$5.7 \times 10^3 - 1.6 \times 10^5$	$v(C_2H) = 0.97$
(0– 79 - 100%)		
$\rightarrow C_2 + H_2$		$v(C_2) = 1.4$
(0– 21 - 100%)		
$C_2H + h\nu \rightarrow C_2 + H$	$5 \times 10^4 - 1.6 \times 10^5$	$v(C_2) = 0 - 2$
$C_2 + h\nu \rightarrow C + C$	$3.3 \times 10^4 - 3.6 \times 10^5$	

Table 2. Derived lifetimes and production rates from the Monte Carlo simulations for Comet P/Halley on December 20, 1985. The C_2H result is based on an assumption that the only parent molecule for C_2H and C_2 is C_2H_2.

Production rate (sec^{-1})	Lifetime (sec) at 1 AU
$C_2H_2 = 1.25 \times 10^{27}$	see Table 1
$C_2H = 1.0 \times 10^{27}$	1– 100
$C_2 = 1.25 \times 10^{27}$	see Table 1

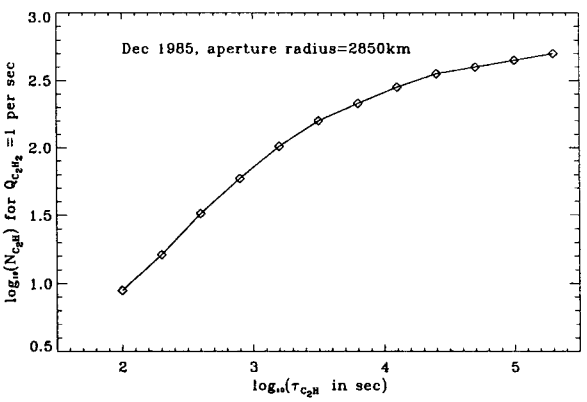

Figure 4.— The number of C_2H molecules within an aperture vs. C_2H lifetime for different observations for Comet P/Halley in December, 1985.

observation by Maillard et al. (1987) was made on December 20.2 and 23.2, 1985, and the C_2 observation by Sivaraman et al. (1987) was made on December 20.6, 1985. Lack of any unusual events in the lightcurve of Comet P/Halley during December 1985, along with the absence of largescale outbursts during these periods of observations has led us to assume a steady-state C_2H_2 production rate. From the C_2 and C_2H observations one can obtain the number of C_2 and C_2H molecules within the observing apertures. The possible lifetimes and velocities of C_2H_2 dissociation products in Table 1 were used. The observations on the number of C_2 molecules within the observing aperture (e.g. Sivaraman et al. 1987) were used to estimate a steady-state production rate of C_2H_2. We derived the C_2H_2, C_2H, and C_2 production rates of 1.25×10^{27}, 1.0×10^{27}, and $1.25 \times 10^{27} sec^{-1}$, respectively, for Comet P/Halley on December 20, 1985. The derived production rates using the Monte Carlo simulations should be more realistic compared with results from the conventional Haser models (Haser, 1957).

Once the C_2H_2 production rate is estimated, one can calculate the number of C_2H molecules within the aperture as a function of C_2H lifetime from the simulations (Figure 4). Comparing the C_2H data with the graphs of C_2H within the aperture versus C_2H lifetime, a reasonable estimate for the C_2H lifetime can be obtained. The acceptable lifetime range is found to be between 1 and 100 seconds. The significant difference between the input lifetime range of C_2H (Table 1) and the obtained lifetime range should be real according to our simulation. In order to obtain the lifetime range, we considered every possible extreme cases of the input parameters listed in Table 1 for the Monte Carlo simulations. Since we assume here that the only parent molecule is C_2H_2, if there are additional sources for C_2H and C_2, then the derived lifetime range is not valid. Table 2 lists our resultant lifetimes and production rates. Using the obtained C_2H lifetime, we constructed a C_2 distribution curve, and compared it with the observed C_2 curves in Figure 2 of O'Dell et al. (1988). Figure 5 shows this comparison. As shown in this comparison, our model that includes a short C_2H

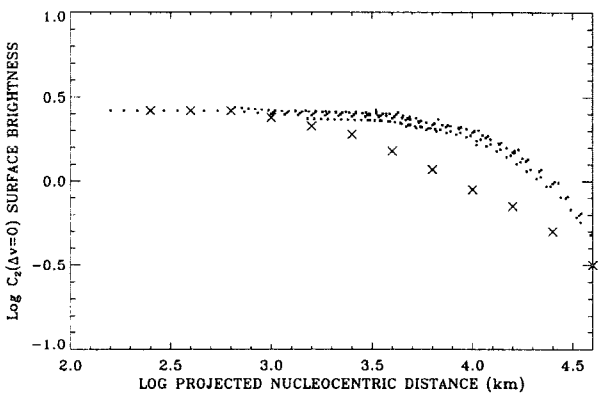

Figure 5.— Dots represent the P/Halley observations of O'Dell et al. (1988). Crosses are the model in which a short lifetime of C_2H is included. It is clear that the difference between the model curve and the observations is large. This leads to a conclusion that there must be significant source(s) for C_2H and C_2 other than C_2H_2.

lifetime clearly does not fit the observed curves. We found that only way to fit the observed curves is to increase the C_2H lifetime significantly, which obviously contradicts the derived range of the C_2H lifetime. We, therefore, conclude that there must be major additional source(s) of C_2H and C_2 other than C_2H_2.

4. CONCLUSION

The small emission peaks at 4010 and 4103 cm^{-1} in the spectra of Comets P/Halley and West coincide with the C_2H band emission peaks. Other emission peaks between 4000 and 4100 cm^{-1} approximately match with the line positions of the $\nu_1 + \nu_3 - 2\nu_2$ band of H_2O. An acceptable lifetime range of C_2H has been derived to be between 1 and 100 seconds at 1 AU heliocentric distance using Monte Carlo simulations, in which we assumed that C_2 and C_2H are produced only from C_2H_2 photodissociation. Based on this assumption, we derived C_2H_2, C_2H, and C_2 production rates of 1.25×10^{27}, 1.0×10^{27}, and $1.25 \times 10^{27} sec^{-1}$, respectively, for Comet P/Halley on December 20, 1985. Using the obtained C_2H lifetime we constructed a C_2 distribution curve and compared it with the observed C_2 curves of O'Dell et al. (1988) to test whether the $C_2H_2 - C_2H - C_2$ reaction is the major reaction chain to produce C_2H and C_2. We found that the difference between the model curve and the observations is large. We, therefore, conclude that there must be significant source(s) for C_2H and C_2 other than C_2H_2.

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