

# Fluorescence efficiencies of the A-X and B-X systems of $\text{CO}_2^+$ in comets

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(Received May 6, 1998; Revised October 9, 1998; Accepted October 20, 1998)

Fluorescence models of the A-X and B-X band systems of  $\text{CO}_2^+$  have been constructed using molecular parameters available in literature. The models have been compared with the spectra of comets Austin (1989c1) and P/Giacobini-Zinner. From the best fit, the fluorescence efficiencies of the A-X and B-X band systems have been derived.

## 1. Introduction

Although the A-X and B-X band emissions of  $\text{CO}_2^+$  appears very strong in the spectra of cometary comae as well as ion tails, these bands have not been investigated in detail. It has been, therefore, difficult to properly identify spectral features of comets in the 2800–4000 Å range, and to derive  $\text{CO}_2^+$  abundances in comets. The B-X bands are usually shown in IUE spectra of comets, and the A-X bands occur in the near-UV and visible spectra obtained from ground-based observations. Festou *et al.* (1982) first confirmed the existence of  $\text{CO}_2^+$  by the presence of the B-X bands at 2890 Å in IUE spectra of several comets. They also showed that several emission features of comet Bradfield (1979X) at 3160, 3260, and 3360 Å, where IUE sensitivity decreases rapidly, are attributed to the A-X bands of  $\text{CO}_2^+$ . However, these emission features are not entirely due to the A-X, especially an emission feature at 3360 Å, where the 0–0 band of the NH A-X band is strong. Later, Feldman *et al.* (1993) recognized that the 3360 Å feature in IUE spectra of several comets is mainly due to the A-X band of NH. The a-c (0–0) band of NH also occurs near 3260 Å. Incidentally, the A-X and B-X bands of  $\text{CO}_2^+$  were also detected in the upper atmosphere of Mars in emission by Mariners 6 and 7 in the late 1960s (Barth *et al.*, 1971).

O'Dell *et al.* (1990) reported spectrophotometric observations of comet Brorsen-Metcalf from 3000 to 3600 Å. In addition to the strong emissions of OH A-X and NH A-X bands, they could identify small emission features of  $\text{CO}_2^+$  at 3380 and 3505 Å, and of CN A-X bands between 3570 and 3590 Å. They also tentatively claimed that weak features near 3255, 3293, 3319, and 3547 Å are attributed to the a-c (0–0) band of NH, A-X band of NCN, A-X band of  $\text{S}_2\text{O}$ , and A-X band of  $\text{H}_2\text{CO}$ , respectively. Two years later, Valk *et al.* (1992) communicated with the author of this paper, and revised part of their tentative claims: the weak features near 3255, 3293, and 3547 Å are primarily due to the bands of  $\text{CO}_2^+$ ,  $\text{N}_2^+$ , and  $\text{CO}_2^+$ , respectively. In this report, we re-examine the spectra based on fluorescence calculations, and compare fluorescence models with spectra of comets Austin

(1989c1) and P/Giacobini-Zinner (hereafter GZ). We discuss results of the model fits, and present the fluorescence efficiencies of the A-X and B-X bands of  $\text{CO}_2^+$ .

## 2. Observations

The comet Austin spectra were obtained with the long-slit Cassegrain spectrograph mounted on the 2.7-m telescope at McDonald Observatory between May 29 and June 3, 1990. Detailed descriptions for the detector, spectrograph, observing condition, and general data reduction processes (sky subtraction and solar absorption line removal) were presented previously by Cochran *et al.* (1990) and Valk *et al.* (1992). The spectrograph, which covered the 3000–3600 Å range, was used in long slit mode with a dispersion of 0.89 Å per pixel. As will be discussed later, a spectral resolution of 1.8 Å was obtained by comparing model spectra with the Austin spectra. The slit length was 154 arcsec. Four spectra were obtained from the nucleus region on four different nights, and the comet spectra were averaged in order to increase signal-to-noise ratio.

The observations of GZ were made at the Kitt Peak 2.1-m telescope with the Intensified Image Dissector Scanner (IIDS) spectrograph on June 20 and 21, 1985. Detailed descriptions for the observations, data reductions, sky subtractions, and calibrations are given in Konno (1987). The IIDS spectrograph covered the 3000–6000 Å spectral range with a spectral resolution of 20 Å. Two spatial locations on the comet were sampled each night: the nucleus and tail. In this paper, we use a tail spectrum taken from 10 arcsec from the nucleus on June 20, 1985, in order to fit the  $\text{CO}_2^+$  model to the spectrum.

## 3. Fluorescence Calculation

The A-X system consists of strong ( $v', 0, 0$ )–( $v'', 0, 0$ ) transitions, and weaker ( $v', 0, 0$ )–( $v'', 0, 2$ ) transitions. The Franck-Condon (F-C) factors for these bands were calculated by McCallum and Nicholls (1971). In McCallum and Nicholls (1972), they compared their values with experimental band strengths observed by several authors, and found that the difference sometimes exceeds a factor of two for weak lines, but the difference is less than 50% for strong transitions (see Table 3 of McCallum and Nicholls, 1972). We used the F-C factors of McCallum and Nicholls (1971), because their

values cover a wide range of vibrational states compared with the experimental intensities, which are not necessarily representing F-C factors (e.g., see an intensity equation in p. 1419 of McCallum and Nicholls, 1972). To our knowledge, upgraded F-C factors are not available in literature.

The rotational line positions of the A-X system are only partially available in the literature. Gauyacq *et al.* (1979) obtained vibrational-rotational constants from high spectral resolution laboratory observations. The relative accuracy of line positions was claimed to be about  $\pm 0.02 \text{ cm}^{-1}$ , but the absolute accuracy is not known. We, therefore, decided not to construct a line-by-line fluorescence model including rotational transitions. For approximate calculations, we only considered vibrational transitions, and this greatly simplifies the calculations. As we mentioned above, the uncertainties in the Franck-Condon factors are up to 50% for strong lines. Thus, detailed line-by-line fluorescence calculations including all the rotational transitions may not be necessary. We used vibrational band head positions measured by Ajello (1971). The uncertainty of the band head line positions is believed to be approximately 1 Å. This uncertainty may be acceptable for our approximate analysis purpose, because the spectral resolutions of comets Austin and GZ spectra are 1.8 Å and 20 Å, respectively. Furthermore, as we discussed in the next paragraph, we can approximately ignore the Swings effects, and, therefore, accurate line positions are not essential in this work.

Table 1 of A'Hearn *et al.* (1983) listed averaged solar radiation densities in a 10 or 20 Å interval. We adopted this table for the calculations of electronic excitations by solar radiation, because of the following reason. The rotational B constant of the A-X system is only  $0.35 \text{ cm}^{-1}$ , and the space between lines in wavenumber is about  $0.70 \text{ cm}^{-1}$ , which corresponds to approximately 0.07 Å. Within a  $v'-v''$  band, there can be as many as 100 rotational lines, and solar flux in the 2800–4500 Å range varies approximately randomly. According to high resolution spectra presented in Fig. 1 of Gauyacq *et al.* (1979), the A-X band widths are less than 10 Å, and the band heads are always on the same side of the bands. We therefore expect that the Swings effects should be approximately cancelled out within a  $v'-v''$  band. Using the averaged solar radiation density for a  $v'-v''$  band, therefore, may not cause significant uncertainty in the Swings effects. We will discuss the Swings effects in the Austin and GZ spectra in the second last paragraph of this section again.

Einstein A coefficients for the  $v'$  states of the A-X band and the entire B-X band were measured and updated by Herran *et al.* (1983). Individual Einstein A coefficient for each vibrational transition,  $A_{v'v''}$ , was calculated using the F-C factors of McCallum and Nicholls (1971). Einstein B coefficients for the vibrational transitions were then calculated from the A coefficients. The B-A transition probability is expected to be almost negligible compared with those of the B-X and A-X transitions, because Einstein A coefficient is proportional to the cube of a band frequency—The B-X, A-X, and B-A bands occur approximately at 34600, 28450, and 6150  $\text{cm}^{-1}$ , respectively.

The B-X system is a highly accumulated band. This band had been studied in detail by Gauyacq *et al.* (1979) and Rostas and Tuckett (1982). Since we are focusing on the fluores-

cence process of the A-X band, we treat the B state as a state in the fluorescence calculations. Since the spatial distribution of CO<sub>2</sub><sup>+</sup> is significantly extended from the nucleus, we can assume that the lifetime is considerably greater than an excitation time by UV, which is approximately 50 seconds. We, therefore, assumed fluorescent equilibrium for the fluorescence processes.

We considered pure vibrational transitions in the X state as follows—Like CO<sub>2</sub>, CO<sub>2</sub><sup>+</sup> is a linear molecule having 3 vibrational modes:  $\nu_1$ ,  $\nu_2$ , and  $\nu_3$ . The  $\nu_1$  vibrational mode is symmetric having no dipole moment, and therefore vibrational transitions are forbidden. This means that we do not have to include  $(v'_1, 0, 0) - (v''_1, 0, 0)$  transitions in the X state [hereafter denoted as  $X(v'_1, 0, 0) - X(v''_1, 0, 0)$ ] for the fluorescence calculations. According to Kawaguchi *et al.* (1985), the  $\nu_2$  and  $\nu_3$  absolute band intensities of CO<sub>2</sub><sup>+</sup> are similar to those of CO<sub>2</sub>. According to laboratory observations in literature, however, CO<sub>2</sub><sup>+</sup> exhibits strong  $A(v'_1, 0, 0) - X(v''_1, 0, 0)$  transitions, and weaker  $A(v'_1, 0, 0) - X(v''_1, 0, 2)$  transitions. Neither  $A(0, v'_2, 0) - X(0, v''_2, 0)$  nor  $A(0, 0, v'_3) - X(0, 0, v''_3)$  transitions have been observed in laboratory. This suggests that we may ignore  $X(v'_1, v'_2, 0) - X(v''_1, v''_2, 0)$ , and  $X(v'_1, 0, v'_3) - X(v''_1, 0, v''_3)$  transitions without significantly compromising the results of the electronic fluorescence efficiencies, which we intend to calculate in this paper. Other combination band intensities between vibrational modes are significantly weak, and therefore we ignored these transitions in the calculations.

A set of 39 simultaneous equations (one for each quantum state) has been constructed. Since we assume a fluorescence equilibrium condition, these equations have been solved by Gaussian elimination to derive equilibrium populations in each quantum level. The equations expressing the fluorescence equilibrium can be found, for example, in Eq. (1) of A'Hearn (1978). Intensities per molecule of each band head were then derived from these populations using the Einstein A coefficients mentioned previously. The resultant intensities were convolved with triangular slit functions: 1.8 Å full-width-half-maximum (FWHM) for the Austin spectrum, and 20 Å FWHM for the GZ spectrum.

The model spectra were primarily compared with observed spectra of comets Austin (Valk *et al.*, 1992) and GZ (Konno, 1987), but the spectra were also checked against the spectra of comets Brorsen-Metcalf (O'Dell *et al.*, 1990) and Kohoutek (O'Dell *et al.*, 1990), although exact comparisons were not performed for the latter spectra. We found notable differences between the models and observations for several lines. If the differences occur consistently in the spectra, especially for Austin and Brorsen-Metcalf, then the differences may not be caused from the lack of Swings effect consideration in this paper, because the heliocentric velocities at the times of the observations of Austin and Brorsen-Metcalf are 32 km/sec and  $-28 \text{ km/sec}$ , respectively. The differences are likely due to the uncertain F-C factors, as mentioned previously in the first paragraph of this section. Therefore, we adjusted several corresponding F-C factors, until the fits are satisfactory within the uncertainty of the observed spectra. The F-C factors are presented in Table 2.

The resultant fluorescence efficiency factors (g-factors) for the A-X and B-X transitions are listed in Table 1.

Table 1. Fluorescence efficiency factors (g-factors) for the band heads of the A-X and B-X systems.

band head (Å)	g-factor (sec <sup>-1</sup> )	band*	v'	v''	band head (Å)	g-factor (sec <sup>-1</sup> )	band*	v'	v''
3505	4.958E-04	1	0	0	3856	5.018E-04	1	1	3
3370	5.559E-04	1	1	0	3696	1.512E-04	1	2	3
3247	1.025E-04	1	2	0	3549	1.727E-04	1	3	3
3133	9.244E-05	1	3	0	3413	1.812E-04	1	4	3
3027	2.537E-05	1	4	0	3179	6.685E-05	1	6	3
2933	1.408E-05	1	5	0	3072	4.262E-05	1	7	3
2884	4.656E-04	5	0	0	4047	5.488E-04	2	0	3
3511	6.894E-04	2	0	0	3871	5.783E-04	2	1	3
3378	6.998E-04	2	1	0	3710	3.646E-05	2	2	3
3254	3.080E-04	2	2	0	3562	2.329E-04	2	3	3
3140	6.205E-05	2	3	0	3427	7.883E-05	2	4	3
3034	2.187E-05	2	4	0	3185	2.358E-05	2	6	3
2936	7.181E-06	2	5	0	3075	2.910E-05	2	7	3
2896	4.656E-04	5	0	0	4095	3.383E-04	3	0	1
3669	3.333E-04	1	0	1	3922	7.328E-05	3	1	1
3517	1.581E-04	1	1	1	3757	7.395E-05	3	2	1
3389	1.865E-04	1	2	1	4109	5.419E-04	4	0	1
3265	1.344E-04	1	3	1	3928	1.283E-04	4	1	1
3150	4.757E-05	1	4	1	3762	1.266E-04	4	2	1
3044	6.279E-05	1	5	1	4051	1.935E-04	1	1	4
2884	4.656E-04	5	0	0	3875	2.786E-04	1	2	4
3674	9.604E-04	2	0	1	3720	1.325E-04	1	3	4
3528	9.945E-05	2	1	1	3565	5.512E-05	1	4	4
3394	1.535E-04	2	2	1	4068	1.831E-04	2	1	4
3270	1.505E-04	2	3	1	3891	1.681E-04	2	2	4
3156	1.234E-04	2	4	1	3580	1.798E-05	2	4	4
3049	3.217E-05	2	5	1	3443	2.316E-05	1	5	4
2896	4.656E-04	5	0	0	4306	1.796E-04	3	0	2
3839	5.360E-04	1	0	2	4108	2.184E-05	3	1	2
3680	1.812E-04	1	1	2	3775	1.434E-04	3	3	2
3534	2.640E-04	1	2	2	3622	1.253E-04	3	4	2
3399	1.180E-04	1	3	2	4322	3.348E-04	4	0	2
3280	4.288E-05	1	4	2	4123	1.483E-04	4	1	2
3165	1.322E-04	1	5	2	3942	5.823E-05	4	2	2
3058	5.947E-05	1	6	2	3775	1.540E-05	4	3	2
2959	3.174E-05	1	7	2	4320	9.783E-05	3	1	3
3852	7.512E-04	2	0	2	4122	2.097E-04	3	2	3
3692	1.370E-04	2	1	2	3942	2.015E-04	3	3	3
3545	2.390E-04	2	2	2	4342	1.237E-04	4	1	3
3413	2.272E-05	2	3	2	4142	1.690E-05	4	2	3
3286	8.340E-05	2	4	2	3961	1.066E-04	4	3	3
3170	5.421E-05	2	5	2	3790	1.069E-04	4	4	3
3063	3.893E-05	2	6	2	3637	5.914E-05	4	5	3
2962	2.169E-05	2	7	2	4340	1.304E-04	3	2	4
3905	3.082E-04	3	0	0	4140	9.138E-05	3	3	4
3741	8.881E-05	3	1	0	4361	7.894E-05	4	2	4
3587	5.524E-05	3	2	0	4160	5.495E-05	4	3	4
3915	3.739E-04	4	0	0	3809	6.794E-05	4	5	4
3749	1.593E-04	4	1	0	3997	9.645E-05	4	5	5
3600	3.328E-05	4	2	0	4384	5.623E-05	4	3	5
4030	1.327E-04	1	0	3	4182	1.915E-05	4	4	5

\*Here, 1, 2, 3, 4, and 5 are representing A<sup>2</sup>Π<sub>3/2u</sub>-X<sup>2</sup>Π<sub>3/2g</sub> (v', 0, 0)-(v'', 0, 0), A<sup>2</sup>Π<sub>1/2u</sub>-X<sup>2</sup>Π<sub>1/2g</sub> (v', 0, 0)-(v'', 0, 0), A<sup>2</sup>Π<sub>3/2u</sub>-X<sup>2</sup>Π<sub>3/2g</sub> (v', 0, 0)-(v'', 0, 2), A<sup>2</sup>Π<sub>1/2u</sub>-X<sup>2</sup>Π<sub>1/2g</sub> (v', 0, 0)-(v'', 0, 2) bands, and B<sup>2</sup>Σ<sub>u</sub><sup>+</sup>-X<sup>2</sup>Π<sub>g</sub> (0-0) band, respectively.

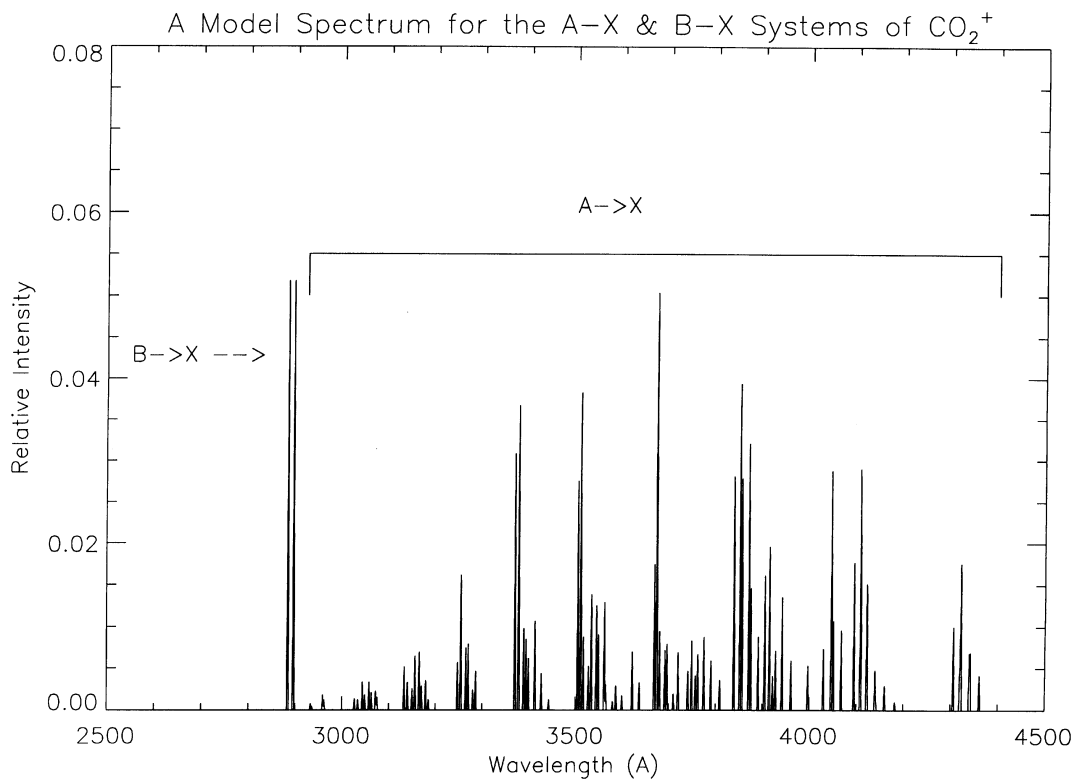


Fig. 1. The best fit model of CO<sub>2</sub><sup>+</sup> A-X and B-X band systems with a spectral resolution of 1.8 Å.

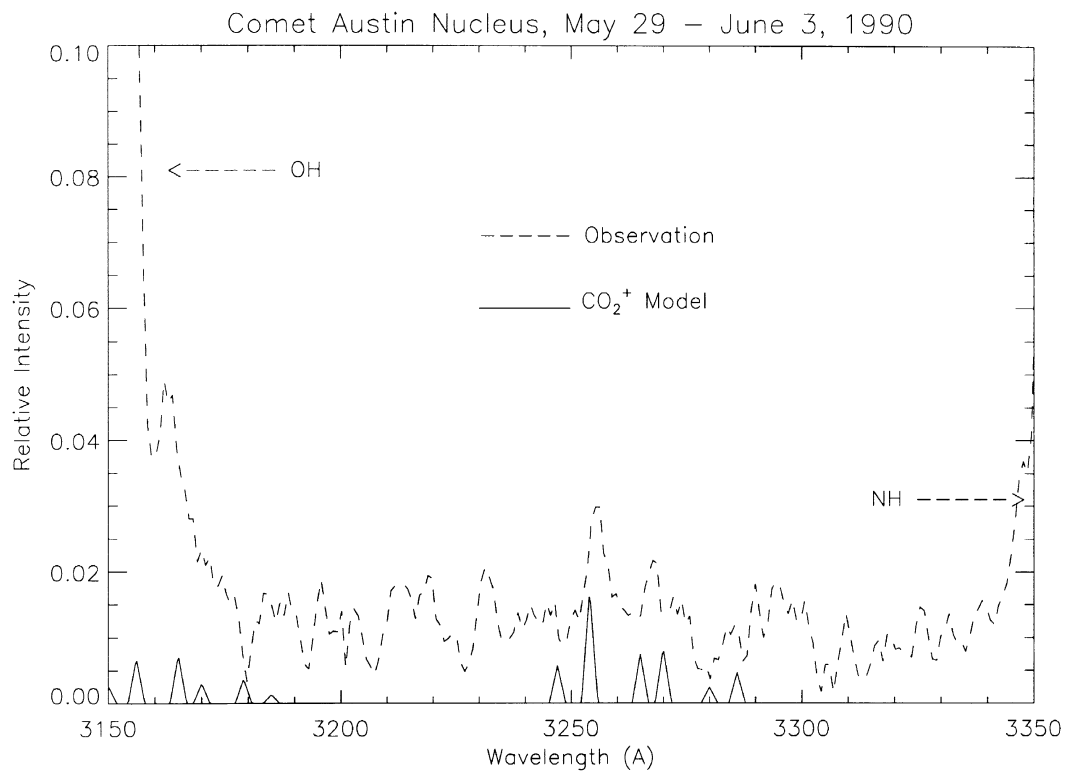


Fig. 2. Comparison between the best fit model and the Austin nucleus spectrum with the same spectral resolution as in Fig. 1. Several weak lines of the model do not match with the small structures in the observed spectra, and this gives an idea for the size of error bars in this figure as well as Fig. 3.

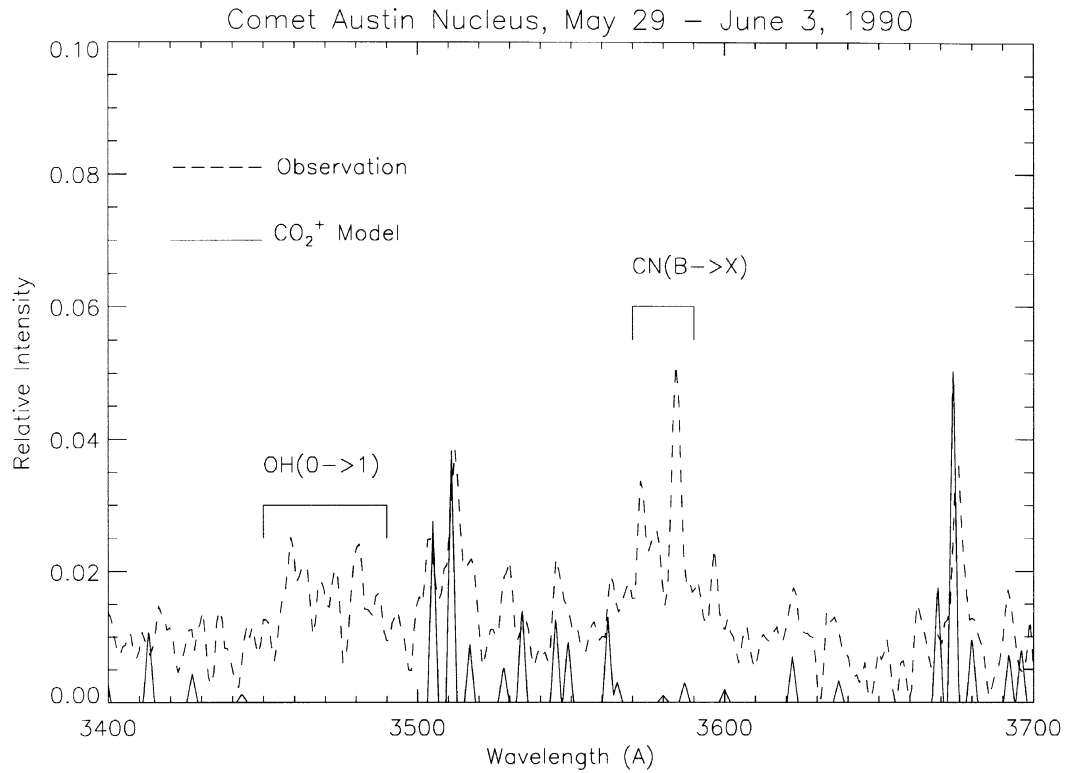


Fig. 3. Another comparison for a longer wavelength range between the best fit model and the Austin nucleus spectrum with the same spectral resolution as in Figs. 1 and 2. OH ( $0 \rightarrow 1$ ) and CN ( $B \rightarrow X$ ) bands are shown.

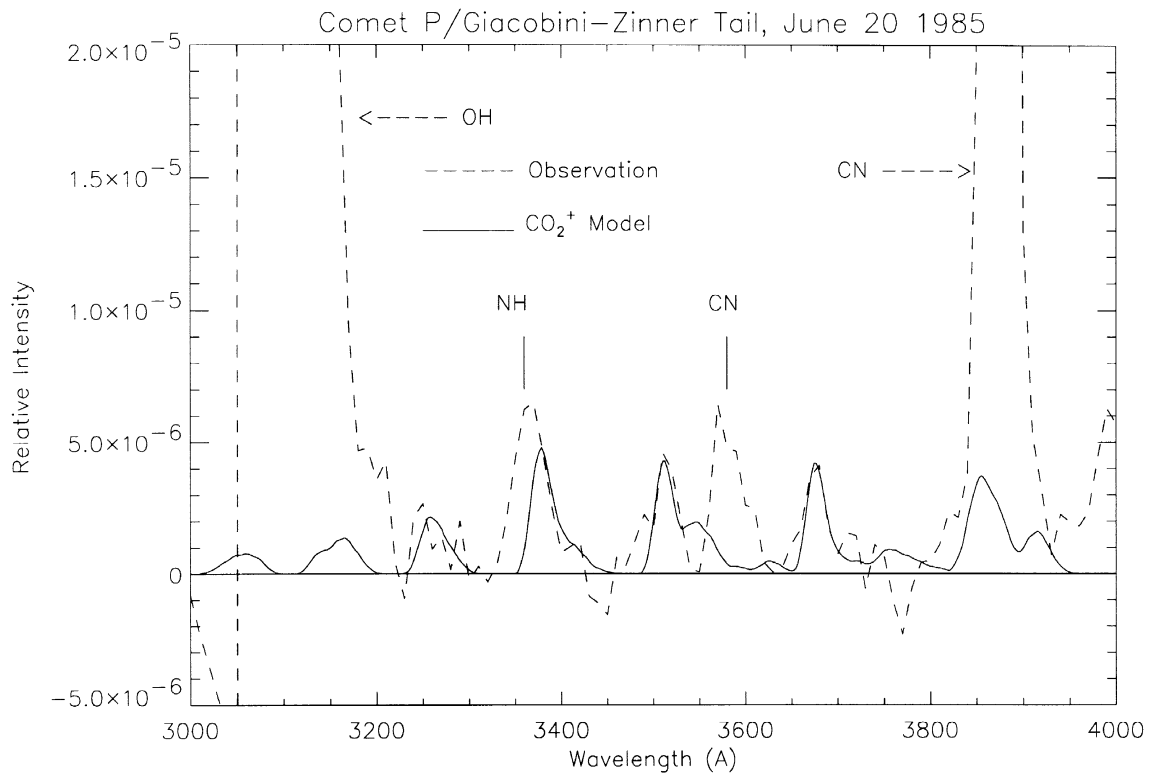


Fig. 4. Comparison of the best fit model and a GZ tail spectrum with a spectral resolution of 20 Å. The NH band is blended with a CO<sub>2</sub><sup>+</sup> band. The negative intensities happen because atmospheric transmission rapidly decreases toward shorter wavelength range, and the negative intensities in the GZ spectrum suggest the degree of uncertainties in the comet spectrum.

Table 2. Franck-Condon factors of the A-X system.

$A^2\Pi_{1/2u}-X^2\Pi_{1/2g} (v', 0, 0)-(v'', 0, 0)$ transitions										
$v' \setminus v''$	0	1	2	3	4	5	6	7	8	9
0	0.23	0.28	0.19	0.12	0.04	0.03				
1	0.40	0.05	0.06	0.22	0.06	0.04	0.03			
2	0.25	0.11	0.15	0.02	0.08	0.08	0.05	0.03		
3	0.07	0.15	0.02	0.18	0.08	0.07	0.21	0.13	0.06	
4	0.04	0.20	0.12	0.10	0.02	0.04	0.06	0.18	0.11	0.02
5	0.02	0.08	0.12	4.E-4	0.14	0.04				
6	6.E-4	0.06	0.13	0.07	0.04	0.04				
7	0.15	0.02	0.10	0.12	0.005	0.04				
$A^2\Pi_{3/2u}-X^2\Pi_{3/2g} (v', 0, 0)-(v'', 0, 0)$ transitions										
$v' \setminus v''$	0	1	2	3	4	5	6	7	8	9
0	0.17	0.10	0.14	0.03	0.04	0.03				
1	0.20	0.05	0.05	0.12	0.04	0.04	0.03			
2	0.05	0.08	0.10	0.05	0.08	0.21	0.05	0.03		
3	0.07	0.09	0.07	0.09	0.06	0.05	0.13	0.02	0.06	
4	0.03	0.05	0.04	0.15	0.04	0.06	0.18	0.11	0.02	0.02
5	0.02	0.08	0.15	0.02	0.04	0.04				
6	6.E-4	0.06	0.13	0.13	0.04	0.04				
7	0.15	0.02	0.10	0.12	0.005	0.04				
$A^2\Pi_{1/2u}-X^2\Pi_{1/2g} (v', 0, 0)-(v'', 0, 2)$ transitions										
$v' \setminus v''$	0	1	2	3	4	5	6	7	8	9
0	0.27	0.34	0.18	0.12	0.04	0.03				
1	0.20	0.14	0.14	0.10	0.06	0.04	0.03			
2	0.06	0.20	0.08	0.02	0.08	0.08	0.05	0.03		
3	0.07	0.20	0.02	0.18	0.08	0.07	0.21	0.13	0.06	
4	0.04	0.20	0.04	0.30	0.02	0.04	0.06	0.18	0.11	0.02
5	0.02	0.08	0.12	0.26	0.26	0.32				
$A^2\Pi_{3/2u}-X^2\Pi_{3/2g} (v', 0, 0)-(v'', 0, 2)$ transitions										
$v' \setminus v''$	0	1	2	3	4	5	6	7	8	9
0	0.23	0.22	0.10	0.03	0.04	0.03				
1	0.07	0.05	0.013	0.05	0.12	0.04	0.03			
2	0.06	0.07	0.08	0.15	0.08	0.21	0.05	0.03		
3	0.07	0.09	0.28	0.23	0.09	0.06	0.21	0.13	0.06	
4	0.03	0.20	0.26	0.23	0.10	0.25	0.06	0.18	0.11	0.02
5	0.02	0.08	0.08	0.15	0.29	0.40				
6	6.E-4	0.06	0.13	0.13	0.04	0.04				
7	0.15	0.02	0.10	0.12	0.005	0.04				

In Fig. 1, we present the best fit model spectrum covering the 2500–4500 Å range. In Fig. 2, a comparison between the model and the Austin nucleus spectrum is presented for the 3150–3350 Å range. In Fig. 3, another model/Austin comparison covering the 3400–3700 Å range is presented. For the model spectra in Figs. 1, 2, and 3, we used a triangular

line profile with a 1.8 Å FWHM. Several weak lines of the model do not match with the small structures in the observed spectra, and this gives an idea for the size of error bars in the Austin spectrum. In Fig. 4, we present a comparison of the model spectrum and a GZ tail spectrum, of which spectral resolution (FWHM) is 20 Å. The tail spectrum is supposed to

have vivid ion emission lines compared with a nucleus spectrum. The NH band is blended with a CO<sub>2</sub><sup>+</sup> band, and a weak CN band is shown near 3570 Å. The atmospheric transmission rapidly decreases toward shorter wavelength range. The negative intensities in the GZ spectrum indicate the degree of uncertainties in the observed spectrum.

#### 4. Discussion

We estimated a rough value for the fluorescence efficiency factor of the NH c-a (0-0) band as follows, in order to clarify the 3255 Å feature in Fig. 4 of O'Dell *et al.* (1990). Valk *et al.* (1992) communicated with the author of this paper, and revised their claim that the 3255 Å is due to a CO<sub>2</sub><sup>+</sup> band, but they did not present a discussion on the revision. The c-X transition is forbidden. The only way to excite the c state seems, therefore, that (1) excitation X → a and then a → c; (2) X → b and then b → c; or (3) it is born to be excited, i.e., photodissociation of its parent molecule (ex. NH<sub>3</sub>) may yield nascent NH (a) state. According to our survey, the nascent NH (a) state and other nascent NH after the NH<sub>3</sub> dissociation are not present in literature. Einstein A coefficient for the a → X transition is greater than 33 /sec, which was adopted from Rohrer and Stuhl (1984). The X → a excitation rate is then estimated to be approximately 8 × 10<sup>-6</sup>/sec. Einstein A coefficient for the b → X transition is ~56 /sec (Huber and Herzberg, 1979). The X → b excitation rate is then estimated to be approximately 2 × 10<sup>-6</sup>/sec. The Einstein A coefficients for the c → a and c → b transitions are 1.85 × 10<sup>6</sup>/sec and 0.21 × 10<sup>6</sup>/sec (Smith, 1969), respectively. Thus, the branching ratio of (c → a)/(c → b) is approximately 9. The corresponding a → c excitation rate is estimated to be approximately 10<sup>-2</sup>/sec, and the b → c excitation rate is less than this value. Therefore, the NH (X → c) excitation rate is estimated to be in the order of 10<sup>-8</sup>/sec, whereas the NH (X → A) excitation rate is approximately 10<sup>-2</sup>/sec (Kim *et al.*, 1989). In summary, the fluorescence efficiency of the NH (c → X) transition is approximately 10<sup>6</sup> times less than that of the NH (A → X). As seen in the observed spectrum (Figs. 2 and 4) of O'Dell *et al.* (1990), the 3255 Å feature is obviously much greater than the 10<sup>-6</sup> times of the NH A-X (0-0) intensity. From the above consideration, we conclude that the feature at 3255 Å is primarily due to the A-X band of CO<sub>2</sub><sup>+</sup>.

We constructed rotational band structures of CO<sub>2</sub><sup>+</sup> using the line-by-line lists of Mrozowski (1941, 1942, 1947) in order to derive a rotational temperature from the Austin spectrum (this model is not presented here). We tested several temperatures, but we could not see discernable changes in rotational structures for different temperatures. Therefore, we could not derive a definite temperature from the 1.8 Å resolution Austin spectrum. As mentioned previously, the space between rotational lines in wavenumber is only about 0.70 cm<sup>-1</sup>, which corresponds to approximately 0.07 Å. Clearly a higher spectral resolution is needed to derive a rotational temperature of the CO<sub>2</sub><sup>+</sup> bands. We defer detailed rotational analysis in our future works.

**Acknowledgments.** I would like to thank Drs. I. Konno and J. H. Valk for kindly providing the GZ and Austin spectra, respectively.

Two referees, Drs. J. Watanabe and D. Schleicher, made several constructive comments, which improved this paper greatly. This work has been supported by a grant (96-07-02-03-01-3) from the Korean Science and Engineering Foundation.

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