

## Research Note

# An attempt to detect the C<sub>2</sub> intercombination transition lines in comet Hale-Bopp

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**Abstract.** In this paper we report the first attempt to detect directly the intercombination transition lines of the C<sub>2</sub> molecule in a comet. Indeed, these transitions play a key role in the C<sub>2</sub> fluorescence process but had never been observed directly so far. We conducted an observational program with the Cerro Tololo Interamerican Observatory 4 m telescope, located in Chile, on September 15<sup>th</sup> and 16<sup>th</sup>, 1997. The spectral range covered was 1.99 - 2.15  $\mu\text{m}$ , in order to detect the emission lines of the  $X^1\Sigma_g^+ - a^3\Pi_u$  (3,0) band, that should be degraded to the blue with a bandhead located at 2.127  $\mu\text{m}$ . This band was chosen because of its expected brightness and its wavelength, corresponding to a good atmospheric transmission and a relatively low sky background. In this paper we present the theoretical calculation allowing to model the expected spectrum and the results obtained with our observational data. These results, unfortunately, cannot allow the detection of the expected emission lines. This is due to a too strong noise, generated by the sky background emission lines, that cannot be totally removed from the spectrum.

**Key words:** molecular processes – comets: general – comets: individual: C/1995 O1 (Hale-Bopp) – infrared: solar system

## 1. Introduction

The C<sub>2</sub> molecule is a well-known species in the cometary spectra, since it appears as one of the brightest features in the visible range. The fluorescence process of this molecule is strongly dependent on some intercombination transitions occurring between the singlet and triplet states. These transitions are normally forbidden by electric dipole radiation, nevertheless their existence is due to higher order multipole radiation and to the perturbations occurring between the different states. The knowledge of these transitions is due, so far, either to theoretical work (Le Bourlot & Roueff 1986) or to a comparison of the “classical spectra” (mainly the Swan bands, appearing around 500 nm) with fluorescence calculations including some intercombi-

nation transitions (Krishna Swamy & O’Dell 1987; Gredel et al. 1989; Rousselot et al. 1994).

The energy levels (see Fig. 1) can be divided in two types of levels: the singlet states ( $X^1\Sigma_g^+$ ,  $A^1\Pi_u$ ,  $C^1\Pi_g$  and  $D^1\Sigma_u^+$ ) and the triplet states ( $a^3\Pi_u$ ,  $b^3\Sigma_g^-$ ,  $c^3\Sigma_u^+$ ,  $d^3\Pi_g$  and  $c^3\Pi_g$ ). The  $a^3\Pi_u - X^1\Sigma_g^+$  transitions play a key-role. Indeed, because of the homonuclear nature of the C<sub>2</sub> molecule, the pure vibrational or rotational transitions are forbidden. Hence the only way for the molecules which are in an excited  $a^3\Pi_u$  or  $X^1\Sigma_g^+$  vibrational state, is either to go to an excited electronic state and come back to a lower vibrational state, or to decay through the  $a^3\Pi_u - X^1\Sigma_g^+$  transitions.

The basic idea used to conduct our observational program is that, even if the transition probabilities of the intercombination transition lines is very weak (about  $10^{-7}$  or  $10^{-8}$  those of the Swan bands, for instance), it can be compensated by the higher relative population levels of the  $X^1\Sigma_g^+$  or  $a^3\Pi_u$  states. A close exam of the expected wavelengths corresponding to the different bands, added to a rough estimation of the expected intensities revealed that the  $X^1\Sigma_g^+ - a^3\Pi_u$  (3,0) band is probably one of the best candidates for a first direct observation of an intercombination band.

## 2. Theory

In order to compute the emission spectrum of the  $X^1\Sigma_g^+ - a^3\Pi_u$  (3,0) band we used a model similar to the one described in a previous paper (Rousselot et al. 1994). This model is a Monte-Carlo simulation based on an initial energy distribution and the time elapsed since the C<sub>2</sub> molecule was created. The levels included are all the rotational levels of the first six electronic states ( $X^1\Sigma_g^+$ ,  $a^3\Pi_u$ ,  $b^3\Sigma_g^-$ ,  $A^1\Pi_u$ ,  $c^3\Sigma_u^+$  and  $d^3\Pi_g$ ) each of them with its six first vibrational states, themselves with all the rotational levels having J inferior or equal to 100. Table 1 summarizes the constants used to compute the energies of the different levels, with the usual notations.

For the triplet states, since there exists three sub-states, some more accurate formulae were used. For the  $a^3\Pi_u$  state the formulae are given by Phillips (1968) (and the constants given in Table 1 by Amiot et al. (1979)). For the  $b^3\Sigma_g^-$  the rotational energies were computed in using the formulae given

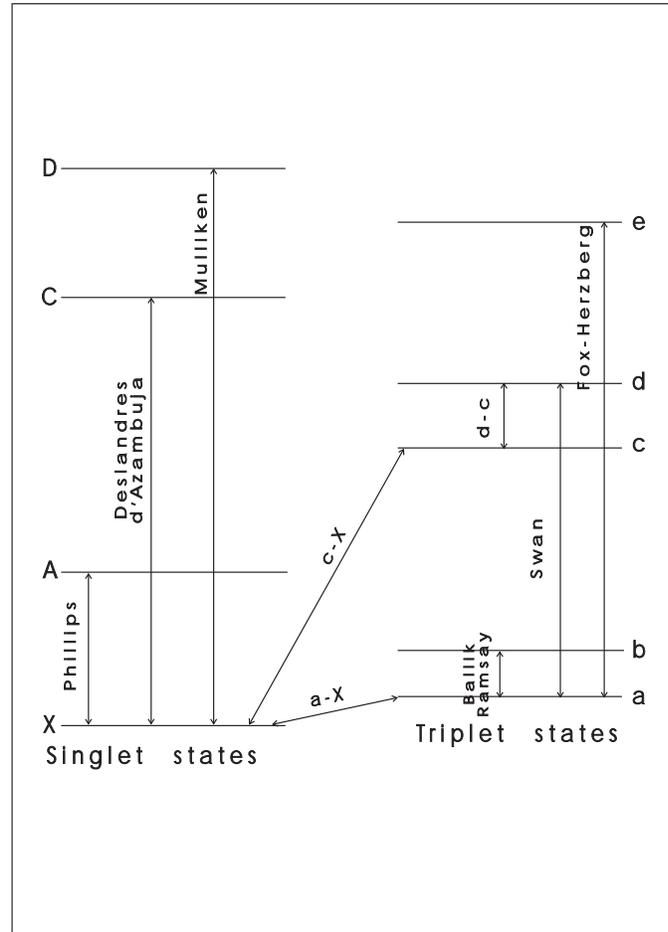
by Amiot et al. (1979) (and the constants given in Table 1 by Ballik & Ramsay (1963)). For the  $c^3\Sigma_u^+$  state the constants given in Table 1 are due to Chauville et al. (1977). For this state, since the energy values are very approximate, we used  $F_1(N) = F_2(N) = F_3(N) = B_e N(N+1)$ . For the  $d^3\Pi_g$  state the constants are due to Phillips (1968), the  $G(v)$  and  $F(J)$  values being calculated with formulae similar to those used for the  $a^3\Pi_u$  state. The data given in Table 1 for the  $X^1\Sigma_g^+$  and  $A^1\Pi_u$  states are due to Chauville et al. (1977). It is important to note that the  $T_e$  value for the  $a^3\Pi_u$  state, which is the key parameter to compute the wavelengths of the  $X^1\Sigma_g^+ - a^3\Pi_u$  bands, was inferred, so far, from the perturbations of some of the rotational energy levels of the  $b^3\Sigma_g^-$  state caused by the  $X^1\Sigma_g^+$  state.

These rotational perturbations were studied first by Ballik & Ramsay (1963) for the vibrational levels  $v=0,1$  and 2 of the  $b^3\Sigma_g^-$  state, giving a  $T_e$  value for the  $a^3\Pi_u$  state of  $716.24\text{ cm}^{-1}$ . A more recent study (Amiot et al. 1979), extended to the vibrational levels  $v=0,1,2,5$  and 6, lead to the  $T_e$  value given in Table 1 (i.e.  $718.3181\text{ cm}^{-1}$ ). The small difference (about  $2\text{ cm}^{-1}$ ) between these two independent results would imply a relatively good accuracy for this value (leading to an uncertainty of only a few Å in the line wavelengths of the theoretical spectrum).

The solar flux values used in the calculations are taken from the NSO/Kitt Peak FTS data given on-line by NSF/NOAO (Kurucz 1984), for the 2960 to 13000 Å range (fluxes averaged to 1 Å intervals) and Thekaekara (1974) above (up to 1 mm, with a stronger smoothing).

The electronic transitions considered are: Phillips ( $A^1\Pi_u - X^1\Sigma_g^+$ ), Ballik-Ramsay ( $b^3\Sigma_g^- - a^3\Pi_u$ ), Swan ( $d^3\Pi_g - a^3\Pi_u$ ),  $d^3\Pi_g - c^3\Sigma_u^+$ ,  $a^3\Pi_u - X^1\Sigma_g^+$  and  $c^3\Sigma_u^+ - X^1\Sigma_g^+$ . The  $A_{v'v''}$  are taken from Gredel et al. (1989) for the Swan system, from Chabalowsky et al. (1983) for the Ballik-Ramsay system, from Van Dishoeck (1983) for the Phillips system (for this system we normalized the  $A_{v'v''}$  values in using an oscillator strength  $f_{00} = 1.5 \cdot 10^{-3}$ ). For the  $d^3\Pi_g - c^3\Sigma_u^+$  transition we have considered a constant ratio  $A_{v'v''}^{d-c}/A_{v'v''}^{d-a} = 0.1$ . Concerning the intercombination transitions, poorly known, we considered an electronic transition moment  $|D_{a-X}|^2 = 2.10 \cdot 10^{-5}$  a.u. and  $|D_{c-X}|^2 = 10^{-4}$  a.u. and some Franck-Condon factors published by Krishna-Swamy and O'Dell (1987) for the  $c^3\Sigma_u^+ - X^1\Sigma_g^+$  transition and kindly provided by Zucconi (1992) for the  $a^3\Pi_u - X^1\Sigma_g^+$  transition. The Hönl-London factors were taken in Le Boulrot (1987) (Phillips and Swan transitions) and Kovacs (1969) for the other transitions.

Since the results given by the Monte-Carlo method are noisy, even with the large number of molecules considered in our calculations ( $9 \cdot 10^5$ ), we decided to smooth the final relative population distribution, both in adding some results obtained at  $t=50000\text{ s}$  and  $t=70000\text{ s}$  (i.e. when the fluorescence equilibrium is reached) and in smoothing the noise in the final population distribution. The result is shown in Fig. 2. This synthetic spectrum shows only the (3,0) bandhead even if, in fact, some much weaker lines, due to the Ballik-Ramsay and Phillips systems, or even to the (4,1) or (5,2)  $X^1\Sigma_g^+ - a^3\Pi_u$  bands, appear in the same region.



**Fig. 1.** Energy level diagram of the C<sub>2</sub> molecule. Each energy level corresponds to the first vibrational state of the respective electronic state.

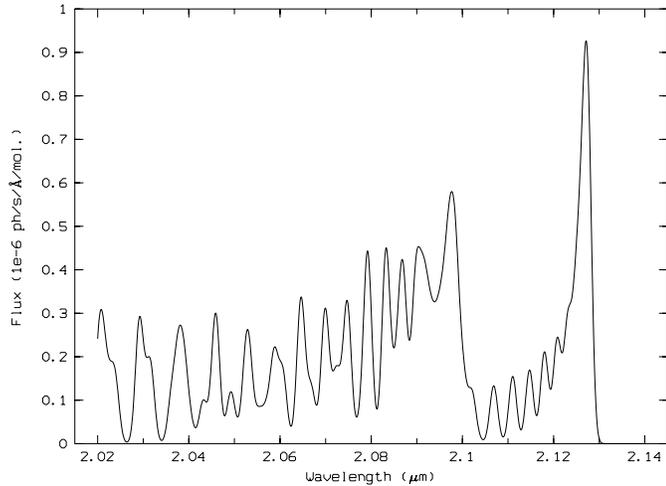
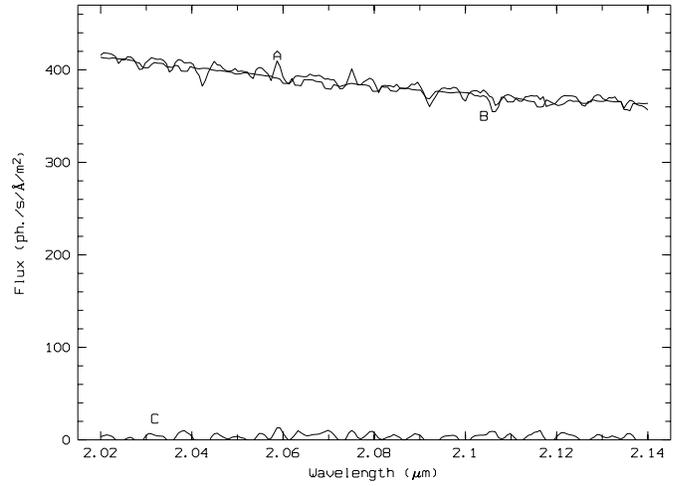
### 3. Observational data

Two half nights, on September 15<sup>th</sup> and 16<sup>th</sup>, 1997 (in the morning) were allocated by the Cerro Tololo Interamerican Observatory (CTIO) to our observing program of Comet Hale-Bopp. This observing run was part of an exchange of 4 m class telescope time between ESO and CTIO and was possible, consequently, thanks to ESO. At this date comet Hale-Bopp heliocentric and geocentric distances were respectively 2.7 and 3.05 AU. Despite this great distance its activity was always important (the whole magnitude was around 5), allowing our attempt to detect the C<sub>2</sub> intercombination lines. The instrument used was the 4 m telescope with the Cerro Tololo Infrared Spectrometer (IRS).

The slit size used was  $0.96 \times 12''$  ( $3 \times 50$  pixels), and its center was located on the nucleus. The detector was a  $256 \times 256$  InSb array, used with a grating of 75 lines/mm and a blaze at  $4.65\ \mu\text{m}$ , giving  $0.00066\ \mu\text{m}/\text{pix}$  at its second order. A k+ filter was used and the spectrometer was centered at  $2.07\ \mu\text{m}$ , giving a spectral range from  $1.986$  to  $2.154\ \mu\text{m}$  and a spectral resolution of  $0.0020\ \mu\text{m}$ .

**Table 1.** C<sub>2</sub> constants used to calculate the energy levels

State	$X^1\Sigma_g^+$	$a^3\Pi_u$	$b^3\Sigma_g^-$	$A^1\Pi_u$	$c^3\Sigma_u^+$	$d^3\Pi_g$
$T_e$	0	718.3181	6435.736	8391.643	9227.4	20024.5781
$\omega_e$	1855.754	1641.3423	1470.415	1608.229	2040.5	
$\omega_e x_e$	14.136	11.66474	11.1549	12.089	14.1	
$\omega_e y_e$			$1.391.10^{-2}$	-0.6		
$B_e$	1.820101		1.4986431	1.616560	1.88	
$\alpha_e(10^{-3})$	18.190		16.3121	16.953		
$\gamma_e$			$-4.61.10^{-6}$	$-4.07.10^{-5}$		
$D_e(10^{-6})$	6.9396		6.1958	6.4895		
$\beta_e$	$+66.9.10^{-9}$		$-6.62.10^{-9}$	$-2.74.10^{-8}$		
$\beta'_e$			$4.78.10^{-10}$			

**Fig. 2.** Synthetic spectrum of the  $X^1\Sigma_g^+ - a^3\Pi_u$  (3,0) band, convolved with a similar instrument response function of IRS (20 Å). The bandhead is located at 2.127  $\mu\text{m}$  (P branch) and the Q and R branches are degraded to the blue.**Fig. 3.** This figure represents the data processing of the final cometary spectrum. A: cometary spectrum, summed over all the spectra and row, without the telluric absorption lines and calibrated in wavelengths and fluxes, B: solar spectrum adjusted to the cometary spectrum and C: A-B (showing only the molecular emission lines, which is reduced here to the noise).

The integration time for each spectrum was 200 s with a typical sequence comet-sky-sky-comet, in order to subtract efficiently the sky background (especially the OH lines). The flat fields were obtained during the day with a dome lamp, the sky spectra were used for the wavelength calibration and the dark current was subtracted in using the overscan region, the spectrum covering only 50 pixels on 256 in x-axis direction.

A bright star (HR 3230) and a spectrophotometric standard (HD 38921) were also observed, in order to compute the transmission efficiency of the earth atmosphere, with a similar spectral resolution, and the absolute fluxes. For both nights a total of 2000 s of integration time could be used, giving a total integration time of 4000 s.

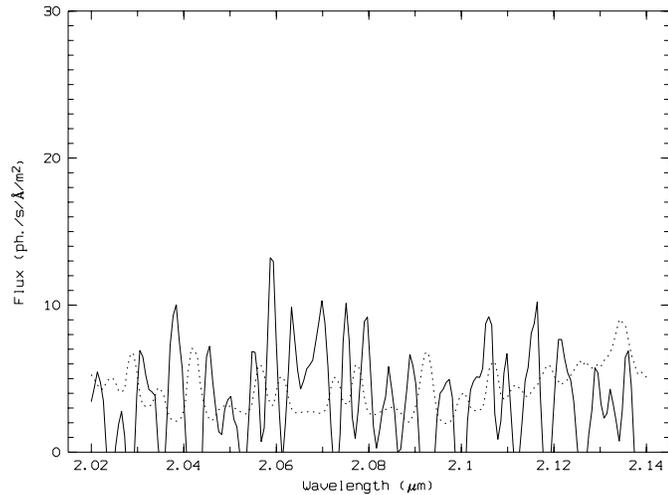
The results are shown in Figs. 3 and 4. Fig. 3 shows the data processing used to subtract the continuum on the cometary spectrum. This continuum is a solar spectrum computed from the NSO/Kitt Peak FTS data produced on-line by NSF/NOAO. These data were smoothed with a similar resolution of the IRS spectrometer. It can be seen that the absorption lines are weak and not really numerous. This spectrum was also adjusted to

the continuum of the cometary spectrum, in order to take into account the effect of the grains scattering. The difference between the cometary spectrum and the solar continuum is shown on the same figure and in Fig. 4, with a more adapted scale. This spectrum represents the final cometary spectrum, showing only the molecular emissions. In this case only the noise is apparent.

#### 4. Interpretation

The comparison of the theoretical spectrum and the experimental data obviously shows that the intercombination band has not been detected. Nevertheless it is important to do a quantitative study, in order to know if this failure is due either to a too high detection limit or to an absence of intercombination bands.

In using the theoretical spectrum it can be seen that the more intense emission lines, with a similar spectral resolution, reach about  $10^{-6}$  ph/s/mol/Å. (it is important to note that this value is not very sensitive to the  $|D_{a-X}|^2$  value, since the relative population levels of the  $X^1\Sigma_g^+$  ( $v=3$ ) state are roughly inversely



**Fig. 4.** The same final spectrum as in Fig. 3 (spectrum C), but with a scale more adapted. The noise can be estimated to about 8 ph./s/Å/m<sup>2</sup>. The spectrum in dashed line represents the sky background (with an intensity divided by 100). It can be seen that, despite a careful data processing to subtract this background, the OH telluric emission lines are often correlated with the final spectrum

proportional to  $|D_{a-X}|^2$ , hence to  $A_{v'v''}$ ). Seen from the telescope the corresponding flux, expressed in terms of ph/s/Å/m<sup>2</sup>, can be computed in using the formula :  $F = 10^{-6} N / (4\pi R^2)$ , where N represents the total number of C<sub>2</sub> molecules appearing in the slit ( $0.96 \times 10^{12}$ ) and R the geocentric distance of the comet (3.05 AU).

The main problem is to evaluate N. This number can be approximated, nevertheless, in using a Haser's model. In using a scalelength for the parent-molecule of 85000 km and another one of 640000 km for the daughter product, with a radial velocity of 0.8 km.s<sup>-1</sup>, it can be computed that, for a production rate of  $10^{28}$  mol.s<sup>-1</sup> (for the parent- molecule),  $N \simeq 5.10^{30}$  molecules. We obtained, consequently, a maximum flux of about 2 ph./s/Å/m<sup>2</sup> for ground-based observations. Since the noise is about 8 ph./s/Å/m<sup>2</sup>, even if the uncertainty on N is high (by a factor 3 or 4) the lack of detection does not contradict the existence of the intercombination lines.

## 5. Conclusion

The failure of this attempt is mainly due to the difficulty to remove completely the sky emission lines. Indeed the statistical noise due to the photons and the read noise of the IRS detector is well below the final noise (it must be below 1 ph./s/Å/m<sup>2</sup>). The problem is also due to a small non-linearity of the CCD detector, difficult to completely correct. Ideally, another attempt to detect these lines should be done outside the earth atmosphere, with a spacecraft (for instance ISO). With a bright comet the S/N ratio would then be dependent nearly only from the photon statistic and, consequently, strongly reduced.

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