EXCITATION MECHANISM OF COMETARY LINES

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The Cometary Spectra in the visible and ultraviolet regions are dominated by the strong emission lines of various molecules. These can be explained in terms of the resonance fluorescence process in the solar radiation.

INTRODUCTION

The cometary spectra in the visible and ultraviolet regions are dominated by emission lines (Swings and Haser 1956, Smith et al 1980, Feldman and Brune 1976). The first step in the study of the spectra is to identify the species responsible for these lines. The second step is to make a quantitative analysis of the spectra in order to get the physical conditions in the source as well as the abundance of the species. However, in order to analyse the spectra, it is essential to know the excitation process of the observed lines. This we discuss here.

EXCITATION PROCESS

Let me first point out a few of the characteristics of the observed emission lines in comets.

The comet gas has a low temperature and the molecules undergo a few or no collisions at all, unless one is very close to the nucleus where densities are higher. The emission spectra of the molecules give different values for the vibrational and rotational temperatures. For example, the molecules CH, CN, etc. give a value of about 50 to 400°K while the C_2 molecule give a value of about 3000°K. The high resolution observation of the CN molecule showed relative intensities of P and R branches of (0, 0) band to be peculiar in showing minimum and maximum intensities at certain locations. This is very different from that of thermal excitation, which gives a smooth distribution of intensities of rotational lines. The observed intensity pattern also depends upon the Sun-Comet distance. It was also found that the details of the intensity pattern observed in two comets are quite different in

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that certain lines were almost absent in one comet while it is strong in the other comet. The emission lines observed arise mostly from the ground electronic state of the molecule, which involve a lot of energy for the excitation of the emission line. This indicates that the excitation of the lines has to be related to the absorption of solar radiation.

All the observed characteristics of the emission lines can be explained by a simple physical process, called the resonance fluorescence process, as was shown in detail by Swings (1941). The absorption of solar radiation in their resonance transitions populates the upper levels, which then trickle down, giving rise to the emission lines.The population in the upper levels depends on the energy available at the wavelength under consideration and this in turn depends upon whether a Fraunhofer line comes in the way of absorption or not. These Fraunhofer lines as seen from the comet have different wavelength shifts depending upon the relative velocity of the comet and the Sun. In fact, Swings showed that there exists one to one relation between the absorbed solar radiation by the molecule and the corresponding emission intensity. This effect is generally known as 'SWINGS EFFECT.'

THEORETICAL ATTEMPTS

The confirmation to the resonance fluorescence process comes from a detailed analysis of the observed and the expected intensities of the rotational and vibrational spectra of molecules (Arpigny 1974, Krishna Swamy 1979, 1981a). Since it is difficult to treat simultaneously the combined effect of vibrational and rotational transitions, they are considered separately for simplicity.

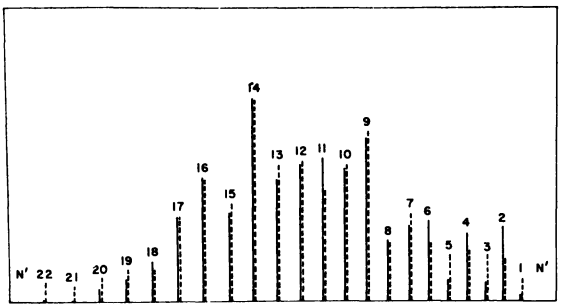

Fig.1. Comparison between the expected (solid lines) and the observed (dashed lines) intensity distribution in the R-branch of the CN violet (0, 0) band of CN in comet Bennett (1970II).

Let us first consider the rotational structure for a given vibrational band. The intensity structure can be calculated provided the population distribution in various rotational levels are known. These in turn can be obtained from the solution of the statistical equilibrium equations of the upper and lower levels for a pure resonance process. A comparison between the relative intensities of the observed and the expected values for the CN (0, 0) band is shown in Fig.1 (Aikman et al 1974, Zucconi and Festou 1985), which shows the validity of the resonance

fluorescence process. Similar agreement is found for other molecules (see Schleicher and A'Hearn 1982).

Let us now consider the vibrational structure of the molecules. Since in general several electronic transitions can arise from the same ground state, they have all to be taken into account along with the vibrational transitions. The solution of the statistical equilibrium equations for the vibrational levels can be used to calculate the expected intensities of vibrational transitions. The expected and the observed intensity ratios for various molecules like CO, CO^+, CS, OH, etc. are in agreement with each other (Arpigny 1964, Krishna Swamy 1979, 1981, 1983a). The synthetic profiles are also in agreement with the observations for comets West and Bradfield (Krishna Swamy 1983a, 1985).

Case of the C_2 Molecule

However, one exception to this general behaviour appeared to be the case of C_2 molecule. It was found that the expected intensities of the Swan band of C_2 molecule were not agreeing with the observed intensities (Stockhausen and Osterbrock 1965, Arpigny 1966, Gebel 1970). Besides the Swan bands arising out of the triplet states are the ones which are strong in the visible region of a cometary spectrum and not those arising out of the singlet ground state.

These problems have finally been resolved based on a detailed modeling of the C_2 molecule, wherein a new physical effect is shown to be very effective in the case of the C_2 molecule (Krishna Swamy and O'Dell 1977, 1979, 1981). This can be understood from the energy level diagram of the C_2 molecule as shown in Fig.2. The C_2 molecule has singlet and triplet states. The Swan bands of the C_2 molecule arise

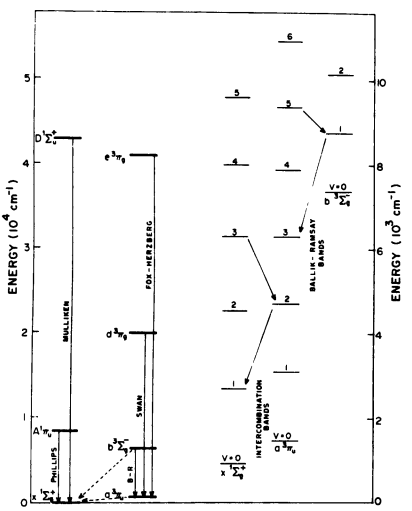

Fig.2. Energy level diagram for the C_2 molecule. The various electronic states are shown on the left-hand side. On the right-hand side are shown the vibrational levels of the three lowest electronic states.

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out of the triplet states, which lies about 714 cm^{-1} higher than the ground singlet state. Fig.2 also shows that vibrational levels of the ground electronic states for v''>4 lies at a higher energy level compared to the energy levels of the next electronic state $b^3\Sigma^-g$. Therefore transition from the higher vibrational levels of $a^3\Pi u$ state can come down to its own lower vibrational levels through the vibrational levels of the $b^3\Sigma^-g$ states as well. The net result is to depopulate the higher vibrational levels of $a^3\Pi u$ state and populating the lower vibrational levels, which result in a non-Boltzmann population distribution. Since C_2 is a homonuclear molecule, the vibrational transitions in the ground electronic states is forbidden. However, the new physical effect as pointed above is in principle equivalent to vibrational transitions. The following system has been considered for the solution of the statistical equilibrium equations: Ballik-Ramsay, Swan and Fox-Herzberg bands of triplet states; Phillips and Mulliken bands of singlet states: singlet-triplet forbidden transitions which is the connecting link between the singlet and triplet states. The resulting Swan band sequence flux ratios are compared with those of observations in Fig.3 and the agreement between the two is satisfactory.

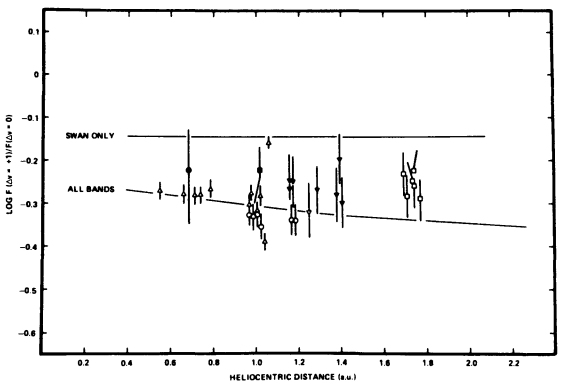

Fig.3. Comparison of the expected and the observed Swan band-sequence flux ratio, $F(\Delta v = +1)/F(\Delta v = 0)$. 'Swan only' refers to earlier work while 'All bands' refers to present work. Points refer to observations of various comets.

These calculations also show that the forbidden singlet-triplet transitions are important. The wavelength of these transitions lies in the infrared spectral region which can be looked for in a cometary spectra as the laboratory analysis of these lines have yet to be made. A by-product of these calculations is that it gave a value for the electronic transition moment, $|Re|^2_{ST}$, for the forbidden singlet-triplet transitions of about 10^{-5}. This value also explains well the observed intensity ratios of the Mulliken/Swan (see A'Hearn and Feldman 1980) and Phillips/Swan bands (Krishna Swamy and C.R. O'Dell 1979, Krishna Swamy 1981b). Several attempts have already been made in recent years to calculate the transition probabilities of the singlet-triplet transitions based on the ab initio methods (Bourlot and Roueff 1986).

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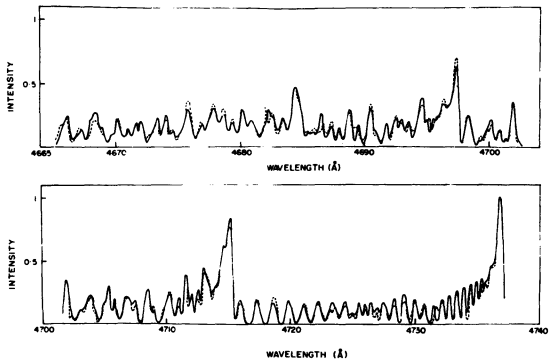

Fig.4. Comparison between the expected (continuous) and observed (dashed) spectra of $\Delta v = +1$ sequence of the C_2 Swan system for comet West.

The next step is to see whether the rotational structure of Swan bands can also be explained by the same mechanism. For this purpose, the statistical equilibrium equations have been solved for the rotational levels of $^3\Pi_0$, $^3\Pi_1$, and $^3\Pi_2$ states of the C_2 molecule. These level populations are used in conjuction with the vibrational population distribution obtained earlier, to calculate the intensities of rotational lines. The synthetic profile is compared with the observed profile of Lambert and Danks (1983) in Fig.4, which show that the rotational structure is also consistent with the resonance fluorescence process (Krishna Swamy 1986).

FORBIDDEN TRANSITIONS

So far we have been considering the allowed transitions. The forbidden doublet lines of oxygen atoms at 6300 and 6364 Å, usually referred to as auroral lines, are very strong in a cometary spectra. The presence of forbidden lines raises the question of their excitation mechanism. It cannot be produced through resonance fluorescence process as the resonance efficiency factors for the red lines are very much smaller than those of ultraviolet resonance lines of 1304 Å (Festou and Feldman 1981). Therefore, resonance fluorescence process cannot be responsible for the excitation of forbidden oxygen lines. It can however be produced through the dissociation of some molecule which leaves them in the levels of interest. They then trickle down giving rise to the emission lines. The potential parent molecule for the oxygen atoms are H_2O and CO_2 (Festou and Feldman 1981, Krishna Swamy and Spinrad 1984).

The resonance lines at 1304 Å also shows some interesting behaviour. The high dispersion spectra of solar line at 1302.2 Å show that for cometary velocities of $\dot{r} \gtrsim 30$ km/sec, the solar absorption wavelength will be completely shifted from the solar line (Feldman et al 1974). However, even for $\dot{r} > 30$ km/sec, the lines of 1304 Å have been seen, which indicate that these lines should be produced by some other mechanism. From the energy level diagram it can be seen that the line of solar

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Lyman β of hydrogen of 1025.72 is very close to the line 1025.77. Therefore the excitation takes place through solar Lyman β induced fluorescence.

Hence, it can be concluded that resonance fluorescence process can explain satisfactorily the intensities of observed emission lines in the ultraviolet and visible spectral regions.

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DISCUSSION

P.K. GHOSH: How much is known about the role of electrons in the excitation process of molecules in comets? Do the internal mode temperatures change with respect to the position of the comet from the Sun? Have there been attempts to sort out the contribution of external photons vis-a-vis cometary electrons in the excitation processes?
KRISHNA SWAMY: The temperature does change with the heliocentric distance. But still they are in the range of a few hundred degrees. At the present time, fluorescence process can explain well all the observations. Only when we have very good high quality data, can one see whether any other mechanism also contributes to the excitation process.

P.D. FELDMAN: In response to question by Ghosh concerning electron excitation: There are certain ultraviolet transitions, such as OI λ 1356, which are not excited by resonance scattering and could serve as indicators of electron excitation in a cometary coma. This transition, as well as some of N_2, have not yet been observed in any comet UV spectrum.

TATUM: The agreement you showed between observed and calculated Swing effect for comet Bennett is pretty good but it may be worth mentioning that in recent months there has been substantial improvement in calculation of cynogen Swing effect.

P.D. SINGH: I would like to make a comment on your slide for comet Bennett (1970 II). The work of Aikman et al. (1974) on fluorescence CN spectrum has recently been improved by J.M. Zucconi and M.C. Festou (Astr. Astrophys. 150, 180, 1985). Zucconi and Festou's theoretical CN fluorescence spectrum calculation gives a better fit to the observed CN (0,0) violet band than Aikman et al. (1974).

ROUEFF: There is a poster paper on ab initio calculations of intercombination transitions in C_2 which takes into account perturbations between $X' \Sigma_g^+$ and $b^3 \Sigma_g^-$ and as well as $a^3\pi_u$ and $A'\pi u$.
KRISHNA SWAMY: The importance of intercombination transitions between the two lowest states $X^1 \Sigma_g^+$ and $a^3\pi_u$ of the C_2 molecule in comets was first pointed out in a paper by the author and O'Dell. In fact, we gave an estimate for the electronic transition moment $|R_e|^2$ for these transitions to be about 10^{-5}, obtained purely from astrophysical considerations. The value could also explain quite well the observed intensity ratios of other band systems. It is therefore, interesting to note that attempts have been made to calculate the transition probabilities of these transitions based on the ab initio method.
It is also worth looking for the infrared lines of singlet-triplet forbidden transitions of the C_2 molecule in a cometary spectrum. If these are detected, it will be the first observation of its kind as the laboratory analysis of these transitions has not yet been made.
OMANT: Is there any polarization observed in cometary lines?
KRISHNA SWAMY: Not yet seen.