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ON THE ROTATIONAL POPULATION DISTRIBUTION OF C_2 IN COMETS

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ABSTRACT

Some of the published general results deduced from the high-resolution spectra of the (0, 0) Swan band of the C_2 molecule from Comet Halley, which should be results common to all comets, are shown to be in qualitative agreement with the results based on time-dependent rotational population distribution.

Subject headings: comets: individual (Halley) — molecular processes

1. INTRODUCTION

The emission bands of the Swan system of the C_2 molecule are the most prominent features in the visible region of cometary spectra. They fluoresce in solar radiation (Krishna Swamy & O'Dell 1977, 1987; O'Dell et al. 1988; Gredel, van Dishoeck, & Black 1989). The observed intensities of the lines should depend upon the physical conditions in the coma as well as on the distance of the comet from the Sun. Because of their high intensity, the Swan bands have been the subject of extensive investigation. In recent years, efforts have been made to secure spectra at higher and higher resolution so as to resolve the rotational structure (Lambert & Danks 1983). A study of these features should help in a better understanding of the physical processes operating in a cometary environment (Gredel et al. 1989).

Comet Halley gave the first unique opportunity for securing good-quality, high-resolution observations of the (0, 0) Swan band over a wide wavelength region (Lambert et al. 1990; Gredel et al. 1989). The beautiful spectra of Lambert et al. were able to resolve the R-branch lines completely. The Boltzmann rotational population distribution derived from these observations has shown several interesting results, which are described in the § 2. In particular, the shape of the observed rotational population distribution in J' appeared to show a steeper dependence for $J' \leq 14$ than for higher J', possibly indicating the presence of two populations corresponding to lower and higher temperatures. Lambert et al. have also remarked that there appears to be no evidence for the presence of a low-temperature component in the rotational structure of the $v' = 2$ level of the Phillips system of the C_2 molecule given the observations presently available. It is, therefore, of interest to investigate whether this feature is unique to Swan bands or should be present in Phillips and Mulliken systems as well. Even though the intensity of the individual rotational lines could vary with the comet, the behavior of the mean rotational spectra over the whole observed spectral region (i.e., J' up to 50 or so) should be a general characteristic feature of all comets. Therefore, our emphasis in the present paper is on the study of this general behavior of the rotational spectra based on the time-dependent rotational population distribution of the C_2 molecule.

2. OBSERVATIONS

The high-resolution spectra of Comet Halley were taken between 1986 March 10 and 1986 April 8. During this period the comet's distance from the Sun varied between 0.85 and 1.29 AU (Lambert et al. 1990). The wavelength coverage of the observation was from 5165 to 5132 Å and the spectral resolution was around 0.06–0.08 (FWHM). The observations were carried out with an entrance slit of size $2'' \times 20''$, centered on the nucleus and, later, on a point $40''$ away from the nucleus in the direction away from the Sun. The spectra has resolved completely the rotational structure and lines up to $P_1(47)$ have been seen. The R-branch lines are also completely resolved. The following interesting features have been deduced from these observations.

The rotational population shows the existence of two different distributions, with the turnover taking place around $J' \sim 15$. The excitation temperatures corresponding to the two populations vary, depending upon the lines used, but are around 600 and 3200 K, respectively. The populations are referred to as cold and hot molecules. The ratio of hot to cold molecules seems to vary slightly with position in the coma, with cold molecules relatively less abundant at $40''$ from the nucleus. The $^3\Pi_2(F_1)$ levels are overpopulated with respect to $^3\Pi_1(F_2)$ for $J' \approx 30$ to 40. The population ratio F_1/F_2 is around 3.0. The F_1 and F_2 levels were unequally populated and F_3 could be underpopulated relative to the F_1 and F_2 levels. For $J' \leq 13$, there is no appreciable population difference between the F_1, F_2, and F_3 levels.

3. MODEL AND CALCULATIONS

Our interest here, as pointed out earlier, is mainly in the study of the general behavior of the rotational structure of the bands of the C_2 molecule, which should be common to all comets, and therefore we can resort to certain approximations. In the present investigation we have considered the transitions arising out of singlet and triplet states simultaneously, unlike our earlier study (Krishna Swamy 1991) in which only the Swan band was considered. In particular, in the solution of the statistical equilibrium equations, we have taken into account the transitions of the Phillips ($A^1\Pi$–$X^1\Sigma_g^+$), Mulliken ($D^1\Sigma_u^+$–$X^1\Sigma_g^+$), Ballik-Ramsay ($b^3\Sigma_g^-$–$a^3\Pi_u$), Swan ($d^3\Pi_g$–$a^3\Pi_u$) and singlet-triplet ($a^3\Pi_u$–$X^1\Sigma_g^+$) systems. In each of the electronic states, five vibrational levels and sixty rotational levels have been taken into account. The substates $^3\Pi_0(F_1)$, $^3\Pi_1(F_2)$, and $^3\Pi_2(F_3)$ existing in each of the triplet states are explicitly considered. These lead to a large total number of coupled equations, around 4500. Some sample calculations were also carried out with some additional levels; we found no appreciable effect on the general nature of our results. The band transition probabilities for the Phillips, Mulliken, and

Ballik-Ramsay systems were taken from Chabalowski, Peyerimhoff, & Buenker (1983) and modified for the recent value of the oscillator strengths of the Phillips and Mulliken systems of Lambert, Sheffer, & Federman (1995). For the Swan system the transition probabilities of Gredel et al. (1989) were used. The band transition probabilities for singlet-triplet transitions have been calculated based on a value for the electronic transition moment of 2.5×10^{-6}, which gives a good fit to the variation of Swan-band flux ratios with heliocentric distance (O'Dell et al. 1988). The Hönl-London factors for the transitions are taken from Schadee (1964). Since the intensity factors for singlet-triplet transitions were not available (Le Bourlot & Roueff 1986), we have used Kovacs's (1969) values. To check the effect of using these values, we also carried out calculations based on the transition probabilities that reproduced the general shape and the total radiative lifetimes of the three substates given by Le Bourlot & Roueff (1986). The wavelengths of the various transitions were calculated using molecular constants (Huber & Herzberg 1979). Since our emphasis in this study is not on the individual rotational lines, but rather on the mean behavior of the rotational population over a wide range of J' values, we were justified in using the smoothed solar radiation field (Krishna Swamy 1981) to describe the incident radiation. The coupled statistical equilibrium equations were solved with the IMSL subroutine DGEAR, which uses the Gear (1971) method of solving time-dependent simultaneous linear equations. The initial population were assumed to be in the lowest rotational level, $v'' = 0$, of the ground electronic state.

4. RESULTS AND DISCUSSION

We have shown in Figure 1 a plot of log $[n(J')/(2J' + 1)]$ as a function of the excitation energy of the level (v', J') for the upper states of the Swan ($v' = 0$), Phillips ($v' = 2$), and Mulliken ($v' = 0$) systems, assuming a typical lifetime for a C_2 molecule of 2×10^4 s before photodissociation. The results are very similar for a lifetime of 2×10^3 s. The figure shows a smooth variation in the rotational population distribution, which steepens for smaller values of the energy. This trend appears to be a general feature for all the substates (Fig. 2). The general nature of the curves for the Swan band can be approximated with excitation temperatures of around 400 and 4100 K, in qualitative agreement with the observations of Lambert et al. The role of singlet-triplet transitions in the change of slope of the Boltzmann diagrams have been discussed by Lambert et al. The general trend in the shape of the curves for the Phillips and Mulliken bands is also quite similar to those for the Swan band. The turnover between the two distributions takes place around $J' \sim 12$ to 16 for the three band systems. Figure 2 shows that for $J' \approx 35$ the ratio of populations $F_1/F_2 \approx 2.1$, comparable to the observed value of 3.0. The difference in the populations between F_1, F_2, and F_3 also decreases with J' for $J' < 13$, consistent with observations. The shape of the curve for F_3 is found to be very similar to that of the curve for F_1.

The general nature of the observed population distribution for the observations carried out on the nucleus and 40″ away from the nucleus is shown in Figure 3. The two curves are made to overlap for large J' values. The shape of the calculated curve is also shown in the figure for two time intervals. The observed and the calculated curves are qualitatively similar. Therefore, the initial rotational populations

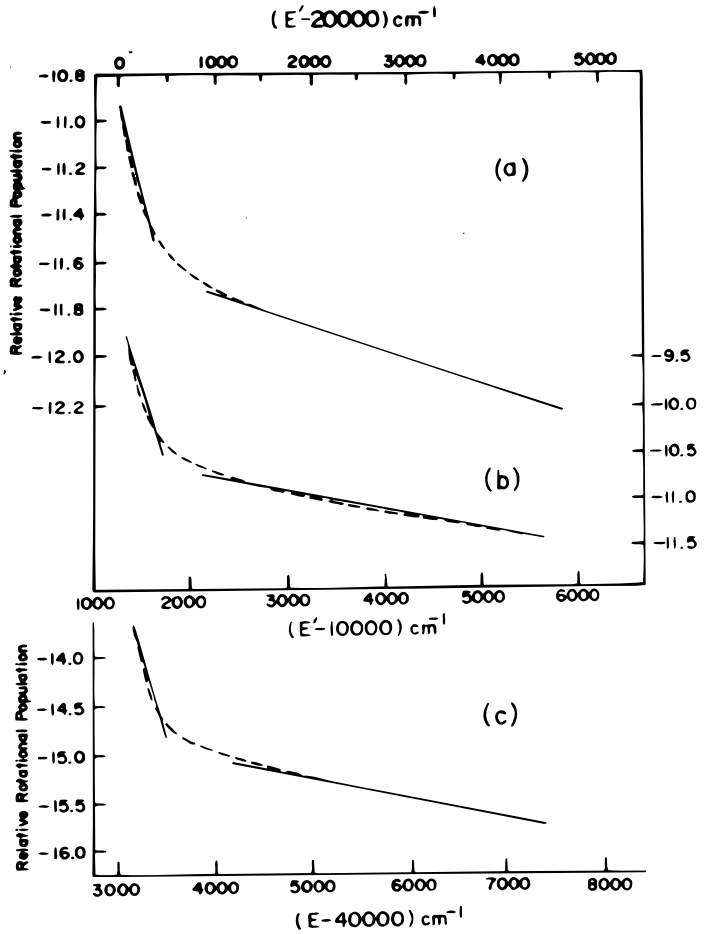

FIG. 1.—Relative rotational population distribution as a function of excitation energy for (*a*) the Swan band, $v' = 0$, (*b*) the Phillips band, $v' = 2$, and (*c*) the Mulliken band, $v' = 0$. The dotted curves show the mean calculated variation at $r = 1.1$ AU. The two straight lines drawn for each curve represent roughly the shape of the curve in the two regions. The excitation temperatures for the Swan band are around 4000 and 500 K, respectively.

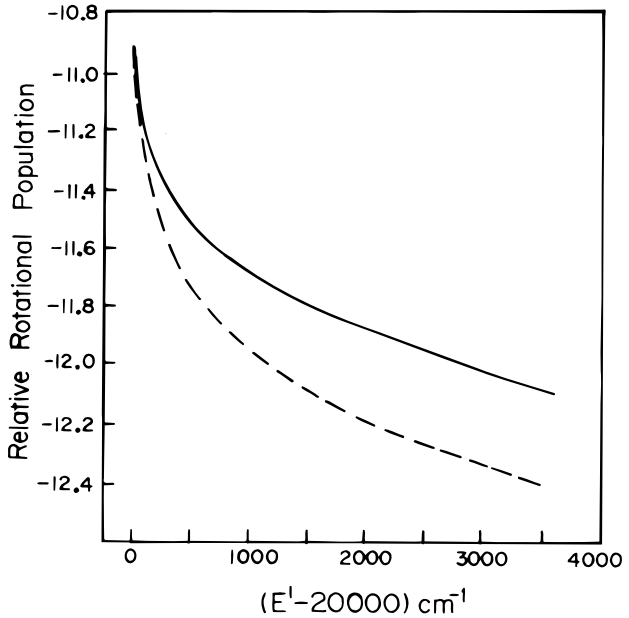

FIG. 2.—Relative rotational population distribution as a function of excitation energy for the substates of the Swan band ($v' = 0$). Continuous and dashed curves refer to F_1 and F_2 states respectively. The curve for F_3 is very similar to the curve for F_1.

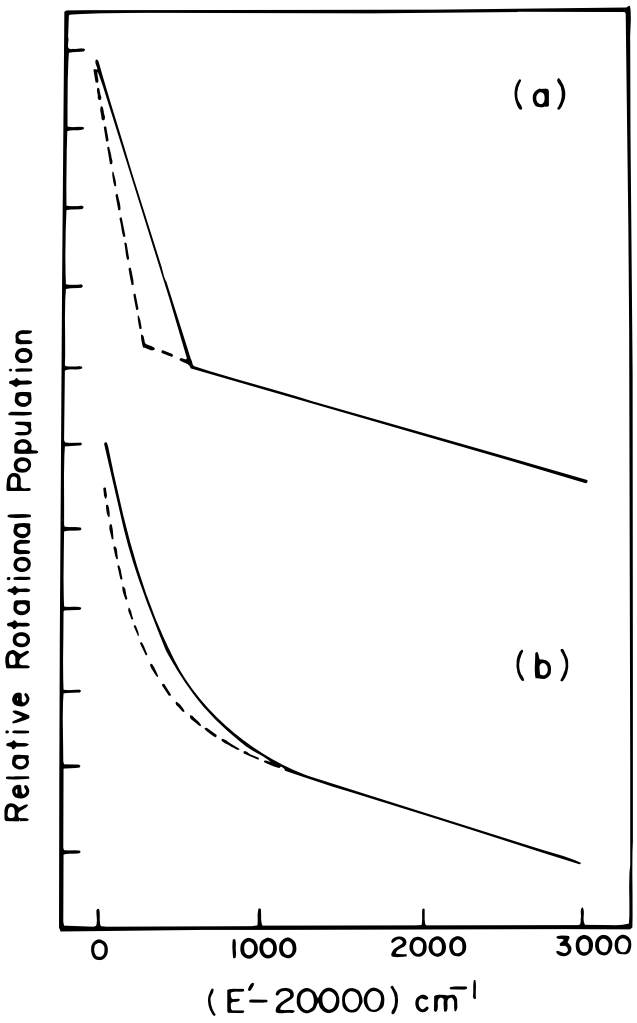

FIG. 3.—Relative rotational population distribution as a function of the excitation energy for the Swan band, $v' = 0$. (*a*) *Continuous lines*: average over the observed populations taken at the nucleus. *Dashed line*: the same, for the data taken at 40″ from the nucleus. The two lines are superposed for large energies (i.e., large J'). (*b*) The calculated rotational population distribution for C_2 lifetimes of 2×10^3 and 2×10^4 s are shown by continuous and dashed curves. The two curves are superposed for larger energies.

arising out of the photodissociation of parent molecules close to the nucleus are gradually erased away from the nucleus as fluorescence cycles produce equilibrium populations (Krishna Swamy 1991).

The inclusion of more vibrational levels, or using the transition probabilities for the singlet-triplet transitions that produce the general shape as well as the total radiative lifetime of Le Bourlot & Roueff (1986), does not make much difference in the qualitative general nature of the curves in Figure 1. The general shape of the variation of population in the rotational levels is also not sensitive to the exact values of the various parameters used. Therefore, in conclusion, the results based on the time-dependent statistical-equilibrium rotational population distribution of the C_2 molecule by the fluorescence excitation mechanism are in agreement with the general results derived from the high-resolution observations of the Swan band.

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