THE LEBLANC BANDS OF THE CN RADICAL IN THE SPECTRA OF COMETS*

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Abstract. Spontaneous emission rates and absorption oscillator strengths for prominent \( \Delta V \leq 4 \) sequence bands of the \( B^2\Sigma^+ \rightarrow A^2\Pi_l \) transition of the CN molecule are estimated. The wavelengths of some lines observed in the coma spectrum of the comet Bradfield 1980t as well as in several comets coincide with these \( \Delta V \leq 4 \) sequence LeBlanc bands of the CN radical. Formation and destruction of the CN radical in the coma of a comet are discussed in the framework of gas phase reactions.

1. Introduction

The CN radical is of major astrophysical importance and has been found to give informations of physical conditions of sources such as comets, stellar atmosphere, and the interstellar medium. In comets, the blue region is dominated by the CN(0, 0) violet band at 3883 Å of the \( B^2\Sigma^+ \rightarrow X^2\Sigma^+ \) transition and Swan bands \( (A^3\Pi_g \rightarrow X^3\Pi_u \) transition) of the \( C_2 \) molecule. The (2, 0) and (3, 1) bands of the CN\( (A^2\Pi_l \rightarrow X^2\Sigma^+) \) red system which appear at 7873 Å and 8067 Å, respectively, were first observed in the comet Mrkos (1957 V) by Swings et al. (1957). Resonance-fluorescence excitation calculations made by Swings and Dufay (1958) and recently by Krishna Swamy (1981) show that the red system is of comparable intensity with the violet system. The CN(2, 0) and (3, 1) bands of the red system have since been observed in the comet 1969g (Tago–Sato–Kosaka) (O’Dell, 1971), comet Kohoutek 1973 XII (A’Hearn, 1975) comet West 1976 VI (A’Hearn et al., 1980). Recently, more bands of the red as well as violet systems of the CN molecule have been observed in the visible spectrum of comet Bradfield (Danks and Dennefeld, 1981; Cosmovici et al., 1982).

The \( B^2\Sigma^+ \) electronic state of the CN molecule can decay radiatively by transitions to the \( A^2\Pi_l \) state \( (B^2\Sigma^+ \rightarrow A^2\Pi_l \) transition) as well as to the \( X^2\Sigma^+ \) state \( (B^2\Sigma^+ \rightarrow X^2\Sigma^+ \) transition). A semi-quantitative laboratory observation by LeBlanc (1968) shows that decay into the \( A^2\Pi_l \) state from vibrational levels 4–9 of the \( B^2\Sigma^+ \) state is only a few percent of that into the \( X \)-state. This conclusion has recently been supported by theoretical calculations made by Larsson et al. (1983) and Cartwright and Hay (1982). The LeBlanc bands of the CN molecule are weaker than the red and violet

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bands and each band forms two sharp heads \((P_2 + Q_{12})\) and \((Q_1 + P_{21})\) separated by about 60 cm\(^{-1}\), which, with moderate inverse dispersion \((-5 \text{ Å mm}^{-1})\) appear as line spectra (LeBlanc, 1968). In this communication, we estimate spontaneous emission rates and absorption oscillator strengths of \(CN(B^2\Sigma^+ + A^2\Pi_i)\) bands and discuss the formation and destruction mechanisms of the CN radical in the coma of a comet. In addition, a comparison of about 30 lines observed in the coma spectrum of comet Bradfield 1980t (Cosmovici et al., 1982) as well as in several comets (Swings and Haser, 1956) with the wavelengths of the LeBlanc band heads show that the \(CN(B^2\Sigma^+ - A^2\Pi_i)\) bands are likely to be present in the coma of a comet.

2. Theoretical Considerations

Duric et al. (1978) have made radiative lifetime measurements of a number of red and violet CN bands at high spectral resolution using the High Frequency Deflection (HFD) technique. They have also reviewed earlier literature on lifetime investigations of the CN radical. The measured absorption oscillator strengths \(f(0, 0)\) of the \((A - X)\) and \((B - X)\) bands of the CN molecule are: \((5.9 \pm 0.6) \times 10^{-3}\) and \((3.11 \pm 0.05) \times 10^{-2}\), respectively. Recently, theoretical investigations of the radiative properties of the CN red and violet systems have been made by Larsson et al. (1983) and Cartwright and Hay (1982). A comparison of theoretical radiative lifetimes for the CN \(B^2\Sigma^+\) state (Table II of Larsson et al., 1983) with those derived by HFD technique (Duric et al., 1978) shows that (i) for \(v' = 0\) and 1, the CASSCF radiative lifetimes (Larsson et al., 1983) are close to HFD lifetimes and (ii) for \(2 \leq v' \leq 5\), ab initio radiative lifetimes are close to lifetimes obtained by Duric et al. (1978). Hence, for \(v' = 0\) and 1 we adopt CASSCF radiative lifetimes and for \(v' \geq 2\) we prefer, \textit{ab initio}, radiative lifetimes of Cartwright and Hay (1982). In Table I, we list these data together with the spontaneous emission rates \(\left(A_{v'} = 1/\tau_{v'} = \Sigma_{v''} A_{v', v''}\right)\) from \(B^2\Sigma^+\) state to \(A^2\Pi_i\) state of the CN radical where (a) electronic branching is allowed and (b) fine structure due to rotation and electron spin has been summed over. Within the framework of realistic Klein–Dunham potential (Jarmain, 1971) for the \(B^2\Sigma^+ + A^2\Pi_i\) states of the CN molecule we have calculated Franck–Condon factors \(q_{v', v''}\) and \(r\)-centroids \(r_{v', v''}\) for \((15 \times 20)\) array of CN\((B^2\Sigma^+ - A^2\Pi_i)\) bands where experimental data of Kotlár et al. (1980) (for \(A^2\Pi_i\) state) and Brocklehurst et al. (1972) (for the \(B^2\Sigma^+\) state) have been used. Using these \(q_{v', v''}\), individual spontaneous emission (transition) rates \(A_{v', v''}\) and absorption oscillator strengths \(f_{v', v''}\) are derived (Schadee, 1978) for \(\Delta V = 1, 2, 3, \) and 4 sequences of the CN\((B^2\Sigma_i - A^2\Pi_i)\) transition and, these values are listed in Table II together with their band origins (in unit of cm\(^{-1}\)) and band heads \(v_{\text{Head}}\) (in units of cm\(^{-1}\) and Å). Each LeBlanc band forms two heads: one due to \((P_2 + Q_{12})\) lines and other by \((Q_1 + P_{21})\) lines. Since splitting is small, \(P_2\) and \(Q_1\) lines lie close to \(Q_{12}\) and \(P_{21}\) lines, respectively. Figures marked by an asterisk in Table II are band heads observed by LeBlanc (1968). Laboratory conditions favor the population of \(v' = 4\text{--}12\) levels of the CN radical in the \(B^2\Sigma^+\) state and, sharp double-headed \(B^2\Sigma^+ - A^2\Pi_i\) bands can be produced with