35. *Vibrational Transition Probabilities of the Phillips System of C₂ Molecules*

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Abstract: Vibrational transition probabilities of Phillips system of C₂ molecules are calculated on the assumption that potential energy curves are approximated by the Morse potential. As 9 upper levels and 5 lower levels of the system have been observed in the laboratory by Ballik and Ramsay (1963), the transition probabilities are calculated for $9 \times 5 = 45$ bands.

Key words: Carbon stars; molecular spectra.

1. Introduction. Recently, sensitivity and accuracy of the observation of stellar spectra have made a rapid progress by the use of Image Intensifier and CCD camera.

In the spectra of Carbon stars CH₂ and HCN lines are identified in these two years by Fujita (1989, 1990).

On the other hand, the study of molecular lines and transition probabilities in the laboratory is not enough.

The Phillips bands of C₂ are observed in the near infrared region of Carbon stars (e.g. V Aql and U Cyg), but the vibrational transition probabilities are not calculated except those by Kamijo (1960) for only four bands.

In this paper transition probabilities are calculated by the same method for bands between 9 upper vibrational levels (${}^1\Pi_u$) and 5 lower vibrational levels (${}^1\Sigma_g^+$). This calculation is very important for the reduction of C₂ spectra of carbon stars, as the accuracy of the observation has been much improved.

2. Method of the calculation. Potential curves of the electronic levels are approximated by the Morse function:

$$(1) \quad U(r) = D[1 - \exp\{-a(r - r_e)\}]^2.$$

Though this function looks very simple, containing only two parameters D and a , the Schrodinger equation for the radial motion of atomic nuclei is solved analytically, and obtained energy levels coincide with experimental results.

3. Summary of the theory. Only simple summary is given in the following. A detailed reduction of the formulae was written by Kamijo (1960).

The boundary condition that wave function vanishes at $r \ll 1$ is fulfilled if $v=0, 1, 2, \dots$ and energy levels are given by

$$(2) \quad \frac{W(K, v)}{hc} = \omega_e \left(v + \frac{1}{2} \right) - x_e \omega_e \left(v + \frac{1}{2} \right)^2 \\ + \left\{ B_e - \alpha_e \left(v + \frac{1}{2} \right) \right\} K(K+1) + D_e K^2 (K+1)^2,$$

where

$$(3) \quad \omega_e = \frac{a}{2\pi c} \sqrt{\frac{2D}{\mu}},$$

$$(4) \quad x_e = \frac{\hbar \omega_e c}{4D},$$

$$(5) \quad B_e = \frac{h}{8\pi^2 \mu r_e^2 c},$$

and

$$(6) \quad \alpha_e = \frac{3\hbar^2 \omega_e}{16\pi^2 \mu r_e^2 D} \left(\frac{1}{a r_e} - \frac{1}{a^2 r_e^2} \right).$$

The left side of Eq. (3)–(6) can be also given by the laboratory experiment.

The Morse parameter D and a are determined by Eqs. (3) and (4). Then, the accuracy of the Morse approximation can be checked by calculating right side of Eq. (6) and comparing with the experimental α_e .

In this case, the accuracy is very good.

The wave function is

$$(7) \quad \Psi_v^v(r) = N_v \frac{1}{r} e^{-z/2} z^{b/2} L_{v+b}^b(z),$$

where

$$(8) \quad L_{v+b}^b(z) = \sum_{k=0}^v \frac{(-1)^k \Gamma(b+v+1)}{k! (v-k)! \Gamma(b+k+1)} z^k,$$

and

$$(9) \quad N_v^2 = ab v! / \Gamma(b+v+1).$$

Now the vibrational transition probability is obtained by square of the overlap integral:

$$(10) \quad \overline{R_{v'v''}}^2 = [I(v', v'')]^2,$$

where

$$(11) \quad I(v', v'') = \int_0^\infty \Psi_{v'}^v(r) \Psi_{v''}^v(r) r^2 dr.$$

From the calculation written above

$$(12) \quad I(v', v'') = \frac{N_{v'} N_{v''}}{a'} \int_0^\infty \exp \left\{ -\frac{1}{2} (z' + \xi z'') \right\} \\ \times z'^{b'/2-1} (\xi z'')^{b''/2} L_{v'+b'}^{b'}(z') L_{v''+b''}^{b''}(\xi z'') dz',$$

where

$$(13) \quad z'' = \xi z',$$

$$(14) \quad \xi = \frac{1}{x_e''} (x_e')^i \exp \{ a'' (r_e'' - r_e') \},$$

and

$$(15) \quad \gamma = \alpha'' / \alpha'.$$

The following molecular constants are used (Herzberg, 1950).

	T_e	ω_e	$\omega_e x_e$	B_e	α_e	$r_e(10^{-8}\text{cm})$	γ_{00}
${}^1\Pi_u$	8391.66	1608.33	12.14	1.6170	0.01720	1.3180	8268.50
${}^1\Sigma_g^+$		1855.63	14.08	1.8205	0.01832	1.2422	

4. Result of the calculation. The obtained $\overline{R_{v'v''}}^2$ are:

$v' v''$	0	1	2	3	4
0	0.412	0.400	0.155	0.0304	0.00321
1	0.331	0.00573	0.292	0.271	0.0863
2	0.162	0.172	0.0564	0.120	0.305
3	0.0632	0.199	0.0330	0.141	0.0203
4	0.0216	0.125	0.139	0.000764	0.157
5	0.00683	0.0597	0.145	0.0603	0.0332
6	0.00205	0.0243	0.0951	0.121	0.0108
7	0.000603	0.00892	0.0490	0.112	0.0764
8	0.000184	0.00304	0.0218	0.0732	0.105

where v' and v'' are vibrational quantum number of the upper level and lower level, respectively.

Generally, it is known:

$$(16) \quad \sum_{v'=0}^{\infty} \overline{R_{v'v''}}^2 = \sum_{v''=0}^{\infty} \overline{R_{v'v''}}^2 = 1.$$

It is very useful to check the numerical calculation. Actually, it holds in every column and in every row of the above table.

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