

FRANCK-CONDON FACTOR FORMULAE FOR ASTROPHYSICAL AND OTHER MOLECULES

R. W. NICHOLLS

Center for Research in Experimental Space Science, York University

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ABSTRACT

Simple closed-form, approximate, analytic expressions for Franck-Condon factors are given. They provide reliable estimates for Franck-Condon factor arrays for molecular band systems for which only ω_e , r_e , and μ_A values are known, as is often the case for astrophysically interesting molecules such as CeO, CoH, CrH, CrO, CuH, GeH, LaO, NiH, SnH, and ZnH for band systems of which Franck-Condon arrays have been calculated.

Subject headings: molecular processes — transition probabilities

I. INTRODUCTION

The Franck-Condon factor,

$$q(v', v'') = \left| \int \psi_{v'}(r) \psi_{v''}(r) dr \right|^2, \quad (1)$$

of a molecular band plays a controlling role in the determination of the relative band intensity and of all the other band transition probability parameters determined by the band strength,

$$S(v', v'') = |\sum R_e|^2 q(v', v''), \quad (2)$$

where $|\sum R_e|^2$ is the sum of the components of the electronic transition moment (Whiting and Nicholls 1974; Whiting *et al.* 1980).

For example, the band oscillator strength is (Nicholls 1969)

$$f(v', v'') = \frac{8\pi^2 m}{3he^2} S(v', v'') \nu(v', v''), \quad (3)$$

where $\nu(v', v'')$ is the band frequency.

Increasing interest in simple molecules in astrophysical environments (e.g., in interstellar space, in stellar atmospheres, and in comets) has emphasized the need for structure and intensity data for such molecules and their transitions (Nicholls 1977). Extensive molecular structure data are available for the more common molecular species (Huber and Herzberg 1979). Such data allow firm identifications of spectral features to be made, and also allow realistic evaluations to be made of molecular potentials, wavefunctions, and such derived quantities of them as Franck-Condon factors. However, for less common, astrophysically important, molecules (e.g., CeO; Wyckoff and Wehinger 1977) the only molecular structure data which exist other than the

reduced mass μ_A are often estimates of the vibrational frequencies ω_e and the equilibrium internuclear separations r_e for a few electronic states (Huber and Herzberg 1979). Diagnostic applications of astrophysical spectra call not only for firm identifications but also for transition probability data, such as Franck-Condon factor arrays, for these molecules too, sparse though the molecular data from them be.

It is thus the purpose of this paper to derive and discuss simple closed-form approximate expressions for Franck-Condon factors based solely on the molecular constants μ_A , ω_e , and r_e . Such formulae for Franck-Condon factors are not only useful for calculation of individual values, and their band-by-band application, but are also useful in studies of radiative transfer in stellar and other astrophysical atmospheres which contain molecular species.

II. THEORY

Many calculations of individual Franck-Condon factors have been made since Franck's (1925) phenomenological and Condon's (1926, 1928) quantum discussions of molecular transitions. They have been reviewed elsewhere (Nicholls 1969, 1977). Such individual calculations are nearly always presented as Deslandres tables of factors, the calculations of which are based on the adoption of a model molecular potential such as simple harmonic oscillator (Condon 1926; Aitken 1951), distorted simple harmonic oscillator (Gaydon and Pearse 1939; Pillow 1949; Nicholls 1950), approximate Morse (Nicholls *et al.* 1960, and earlier papers cited therein), Morse (Nicholls 1965*a*, and earlier papers cited therein), Jarmain, and Nicholls and realistic numerical Klein-Dunham and Rydberg-Klein-Rees potentials (McCallum 1970). The most accurate factors are those based on realistic numerical potentials derived directly from measured molecular constants such as B_v (which

require very careful rotational analyses and critical assessment of input data to delineate the turning points of the classical oscillator for each vibrational level). Nevertheless, comparison between Franck-Condon factors based on realistic potentials, and those based on Morse potentials often reveal remarkable agreement, particularly at low vibrational quantum numbers.

A large data base of Franck-Condon factors developed by the author and his collaborators, stimulated an investigation of the systematics of the arrays and their surfaces, and of interpolation between them using an interpolation parameter which takes a characteristic value for each band system in question (Nicholls 1956, 1965*b*, 1973). The gross overlap between the pair of molecular potentials involved is the controlling parameter which determines the general form of a Franck-Condon factor array, for it controls the amount of overlap between the wave functions of equation (1). The overlap between potentials is controlled by the relative width of the potentials (defined appropriately) and $|\Delta r_e|$, the magnitude of the difference between their equilibrium internuclear separations. In earlier interpolation studies (Nicholls 1956, 1965*b*), a transition parameter t was empirically adopted, which incorporates the anharmonic vibrational constant $\omega_e x_e$. Here

$$t = \bar{\beta} \Delta r_e, \quad (4a)$$

where

$$\beta = (\mu_A \omega_e x_e)^{1/2}. \quad (4b)$$

The notation is standard (Herzberg 1950), and β is part of the exponent of the Morse function. Its average value between the two electronic states involved is used in equation (4a). The quantity t was shown to be a good transition parameter for interpolation purposes (Nicholls 1956, 1965*b*). It was further shown (Nicholls 1965*b*) to have an approximate theoretical basis in the overlap between the relative widths of Morse potentials at half well depth.

In the current work a simpler transition parameter,

$$t = \bar{\beta} \Delta r_e, \quad (5a)$$

is used, where

$$\beta = (\mu_A \omega_e)^{1/2}, \quad (5b)$$

and $\bar{\beta}$ is a suitable mean discussed below. When defined through equations (5a) and (5b), t is a measure of the amount of overlap of potentials at the level $v=0$. If W_1 and W_2 are the respective half-widths of the potentials at their lowest vibrational level, the overlap D between the potentials at $v=0$ is

$$D = W_1 + W_2 - \Delta r_e. \quad (6a).$$

At low vibrational quantum numbers, molecular potentials are quasi-parabolic. The half-width W at $v=0$ for such a potential is

$$W = (h/4\pi^2 c \mu_A \omega_e)^{1/2} = 5.807/(\mu_A \omega_e)^{1/2} = 5.807/\beta. \quad (6b)$$

W is in angstrom units if ω_e is in cm^{-1} , and μ_A is in amu.

If, as an approximation, W_1 and W_2 of equation (6a) are replaced by their average, \bar{W} , equation (6a) may be rewritten to represent a dimensionless overlap P between potentials at $v=0$,

$$P = D/\bar{W} = 2 - \Delta r_e/\bar{W} = 2 - \bar{\beta} \Delta r_e/5.807 \quad (6c)$$

The "average" $\bar{\beta}$ implied in equation (6d) and also in equation (5a) is thus that value of β appropriate to \bar{W} .

That is, from equation (6b),

$$\bar{\beta} = (\mu_A \tilde{\omega}_e)^{1/2}, \quad (6d)$$

where

$$\tilde{\omega}_e^{1/2} = \frac{1}{2}(\omega_1^{-1/2} + \omega_2^{-1/2}) = (\omega_1 \omega_2)^{1/2} / (\omega_1^{1/2}), \quad (6e)$$

and $\omega_1 = \omega'_e$ and $\omega_2 = \omega''_e$ (Herzberg 1950).

Equations (5a) and (6c) imply

$$P = 2 - t/5.807 = 2 - S, \quad (6f)$$

and thus the transition parameter t , as defined through equations (5a), (5b), (6d), and (6e), and the parameter S defined in equation (6f) are good measures of overlap between potentials.

In the following discussion it will be shown that S and $u = S^2/2$ are also good independent variables in terms of which to develop closed expressions for Franck-Condon factors.

We assume that the only band system data which are available are μ_A , ω'_e , r'_e , ω''_e , r''_e . This forces the adoption of a parabolic (simple harmonic oscillator) model of molecular potentials for small vibrational quantum numbers. The basis of the approximation is then to replace the above molecular data by μ_A , $\tilde{\omega}_e$, r'_e , $\tilde{\omega}_e$, r''_e . That is, the two new potentials have equal half-widths \bar{W} at $v=0$, in the spirit of equation (6e).

Each of the wavefunctions of equation (1) is then of the form

$$\psi_v(x) = N_v H_v(x) \exp(-\frac{1}{2}x^2), \quad (7a)$$

where

$$x = (r - r_e) / \bar{W}, \quad (7b)$$

and

$$N_v = (2^v \bar{W} v! \sqrt{\Pi})^{-1/2}. \quad (7c)$$

\bar{W} is the potential half-width at $v=0$, as in equation (6c), and $H_v(x)$ is the Hermite polynomial: $H_0(x)=1$; $H_1(x)=2x$; $H_2(x)=4x^2-2$; $H_3(x)=8x^3-12x$.

The Franck-Condon factor of equation (1) is then

$$q(v', v'') = (N_{v'} N_{v''})^2 I^2(v', v''), \quad (8a)$$

where

$$I_{v'v''} = \int_{-\infty}^{\infty} H_{v'}(x') H_{v''}(x'') \exp \left[-\frac{1}{2} (x'^2 + x''^2) \right] dr. \quad (8b)$$

The x 's are defined equation (7b) with $r_e = r'_e$ or r''_e .

Following the suggestions of Morse (1929), ter Haar (1946), and Mulliken (1939), the limits of the integral of (8b) are taken between $\pm\infty$ rather than between 0 and ∞ .

After some elementary manipulation it is easy to show that equation (8b) can be rewritten as

$$I_{v'v''} = \bar{W} \exp(-S^2/4) \times \int_{-\infty}^{\infty} H_{v'}(\sigma \mp S/2) H_{v''}(\sigma \pm S/2) \exp(-\sigma^2) d\sigma, \quad (8c)$$

where

$$S = \Delta r_e / \bar{W} = t / 5.807, \quad (8d)$$

and

$$\sigma = [r - (r'_e + r''_e)/2] / \bar{W}, \quad (8e)$$

and the upper and lower sign alternatives in the Hermite polynomials depend, respectively, upon whether $r'_e >$ or $< r''_e$.

The polynomial nature of the integrand of equation (8c) reduces the integral to sums and differences of integrals of the form

$$J(2p) = \int_{-\infty}^{\infty} x^{2p} e^{-x^2} dx = \Gamma\left(p + \frac{1}{2}\right) = \frac{1.3.5 \dots (2p-1) \sqrt{\Pi}}{2^p}, \quad (9a)$$

and

$$J(2p+1) = \int_{-\infty}^{\infty} x^{2p+1} e^{-x^2} dx = 0. \quad (9b)$$

Thus, only even polynomial components of the integrand of equation (8c) make a contribution. Using equations (7c) and (8c) it is then possible to rewrite equation (8a) as

$$q(v'v'') = \frac{\exp(-S^2/2)}{(2^{v'+v''} v_1! v_2! \Pi)} K^2(v'v''), \quad (10)$$

where $K(v'v'')$ is the integral of equation (8c).

It is easy to demonstrate that $K(a, b) = K(b, a)$ and thus that there is a symmetry about the prime diagonal ($v' = v''$) of the Deslandres array of Franck-Condon factors in this approximation. Thus, only one of the two sign alternatives of equation (8c) need be evaluated for $q(a, b) = q(b, a)$.

Equation (10) is the general closed form approximate analytic expression for Franck-Condon factors as a function of S (and thus of t and $u = S^2/2$), which we show below has many potential applications. Using equations (9a) and (9b), elementary evaluation of $K(v', v'')$ leads to the specific expressions for $q(v', v'')$ in that part of the Deslandres table which includes $0 \leq v', v'' \leq 3$ displayed in Table 1.

III. RESULTS AND DISCUSSION

Figures 1, 2, and 3, respectively, display plots of $q(v', v'')$ as a function of S and t , calculated from the equations of Table 1, for the v' or $v'' = 0$ progressions, for the $\Delta v = 0$ sequence, and for the (1, 2), (2, 1), (1, 3), (3, 1), (3, 2), and (2, 3) bands. The $q(v', v'')$ values can either be read directly from the plots, or calculated from the equations of Table 1.

The systematic variation of the $q(v', v'')$ values with transition parameter already noted in empirical examination of individually calculated Morse values for 85 band systems (Nicholls 1965b) is confirmed in Figures 1, 2, and 3.

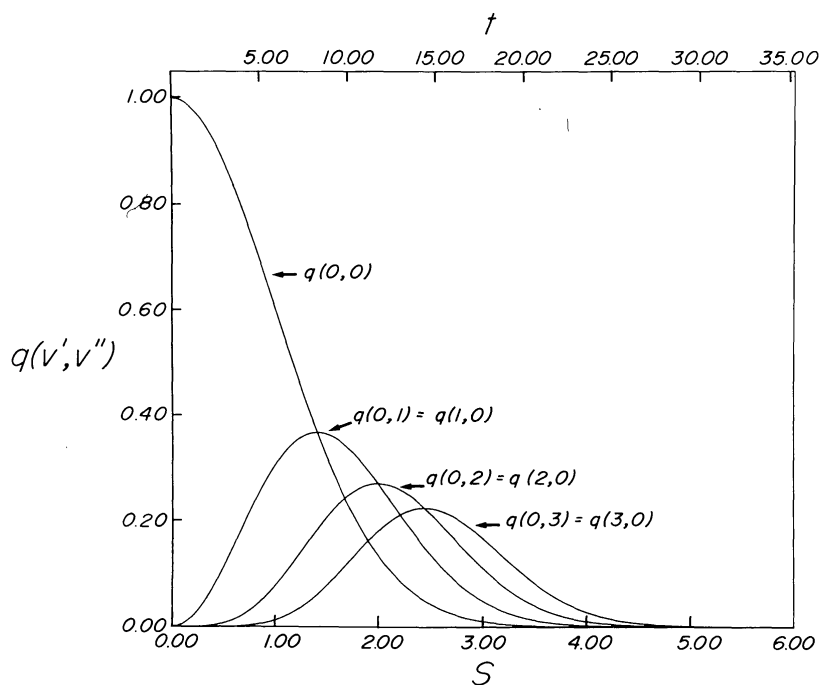
The Franck-Condon factor surface expands smoothly from a sharp diagonal ridge when $S \leq 0.25$, whose peak is at (0,0), through a series of nested ridges for which $q(0,0)$ is the vertex, where the sequences $\Delta v = \pm 1$ play increasingly important roles when $S \leq 1$, to broad nested ridges, symmetrical about $\Delta v = 0$, which avoid (0,0) when $S > 3$. The plan view of these ridges on the (v', v'') plane are the well-known Condon loci.

The variation of any individual Franck-Condon factor with change of S or t , illustrated in Figures 1, 2, and 3, can be likened to the oscillation of a "floater" at the

TABLE 1

FRANCK-CONDON FACTOR FORMULAE FOR THE $0 \leq v', v'' \leq 3$ ARRAY OF BANDS

| | |
|--|---|
| $q(0,0) = \exp(-S^2/2)$ | $q(2,2) = \frac{[(S^2-4)^2-8]^2}{64} \exp(-S^2/2)$ |
| $q(0,1) = q(1,0) = (S^2/2) \exp(-S^2/2)$ | $q(2,3) = q(3,2) = \frac{S^2(S^4-12S^2+24)^2}{384} \exp(-S^2/2)$ |
| $q(0,2) = q(2,0) = (S^4/8) \exp(-S^2/2)$ | $q(2,V) = q(V,2) = u^{V-2} e^{-u} [(u-V)^2 - V]^2 / 2! V! \quad V \geq 2$ |
| $q(0,3) = q(3,0) = (S^6/48) \exp(-S^2/2)$ | $q(3,3) = \frac{\{S^2[(S^2-9)^2-9]-48\}^2}{2304} \exp(-S^2/2)$ |
| $q(0,V) = q(V,0) = u^V e^{-u} / V! \quad V \geq 0$ | $q(3,V) = q(V,3) = u^{V-3} e^{-u} \{(u-V)^3 - V[3(u-V)+2]\}^2 / 3! V! \quad V \geq 3$ |
| $q(1,1) = \frac{(S^2-2)^2}{4} \exp(-S^2/2)$ | |
| $q(1,2) = q(2,1) = \frac{S^2(S^2-4)^2}{16} \exp(-S^2/2)$ | |
| $q(1,3) = q(3,1) = \frac{S^4(S^2-6)^2}{96} \exp(-S^2/2)$ | |
| $q(1,V) = q(V,1) = u^{V-1} e^{-u} (u-V)^2 / V! \quad V \geq 1$ | |

NOTE.— S is the transition parameter $(\mu_A \bar{\omega}_e)^{1/2} \Delta r_e / 5.807$, $u = S^2/2$.FIG. 1.—Dependence of $q(v', v'')$ upon S and t for the $v'=0$ and the $v''=0$ progressions of bands

(v', v'') location on the q -surface as it opens out and the ridges and valleys pass across (v', v'') . It is noted that each of the curves of Figures 1, 2, and 3 exhibit $(v_{\min} + 1)$ maxima, where v_{\min} is the smaller of the two v values involved. Maxima at $S=0$ of $q(v, v)$ are included in this statement.

The equations of Table 1 are remarkably simple and easy to evaluate. It is noted that each of the equations is

of the form

$$q(v', v'') = g(v', v'') q(0, 0). \quad (11)$$

To illustrate the ability of the equations of Table 1 to provide good estimates of Franck-Condon factor values which can be used with confidence in applications, a comparison is made in Table 2 between accurate, realistically calculated values of Franck-Condon factors for

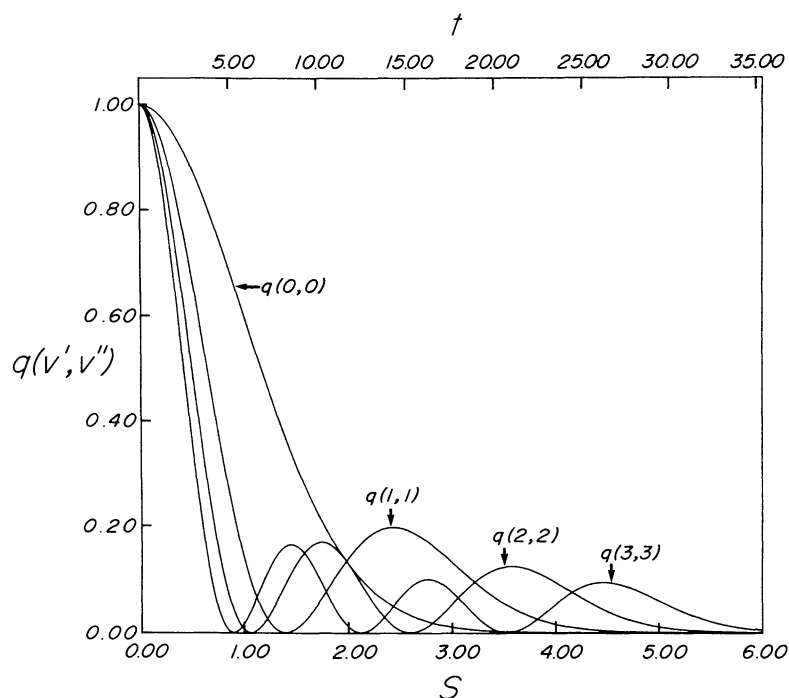


FIG. 2.—Dependence of $q(v', v'')$ upon S and t for the $\Delta v=0$ sequence of bands

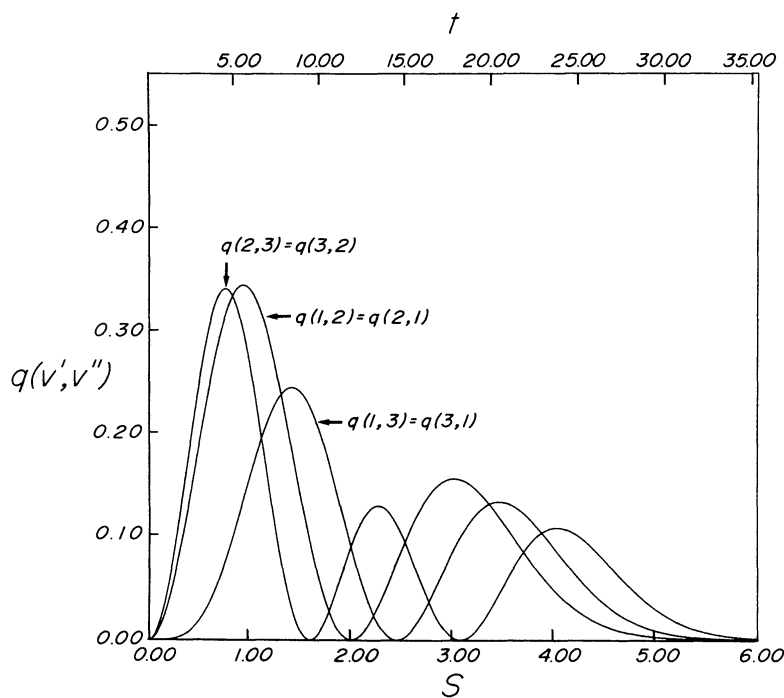


FIG. 3.—Dependence of $q(v', v'')$ upon S and t for the (1,2) and (2,1), (1,3) and (3,1), and (2,3) and (3,2) bands

TABLE 2
COMPARISON BETWEEN REALISTIC FRANCK-CONDON FACTORS OF McCALLUM *et al.* (1970)
(upper entry) AND THOSE CALCULATED BY THIS PAPER (lower entry)
FOR THE A10($B^2\Sigma-X^2\Sigma$) BAND SYSTEM

| v'' | v' | | | |
|---------|-------------------------------|------------------|------------------|------------------|
| | 0 | 1 | 2 | 3 |
| 0 | 7.23-1 ^a 7.18-1 | 2.43-1 2.38-1 | 3.21-2 3.93-2 | 1.86-3 4.35-3 |
| 1 | 2.27-1 2.38-1 | 3.37-1 3.21-1 | 3.53-1 3.31-1 | 7.72-2 9.35-2 |
| 2 | 4.31-2 3.93-2 | 3.02-1 3.31-1 | 1.33-1 1.11-1 | 3.85-1 3.37-1 |
| 3 | 6.22-3 4.35-3 | 9.55-2 9.35-2 | 2.96-1 3.37-1 | 3.76-3 1.96-2 |

^aThe negative number is the power of 10 by which the entry is multiplied. For this band system, $S=0.814$, $t=4.73$, $u=0.331$.

the A10($B-X$) system, based on best molecular data, calculated by McCallum, Jarman, and Nicholls (1970) and the values calculated for the same bands, using the same input data, to the equations of Table 1.

The ω_e , r_e , and μ_A values used in both sets of A10 calculations are those displayed in the first entry of Table 3. In Table 2 the upper entry in each case is the realistic value calculated by McCallum *et al.*, and the lower entry in each case has been calculated by the methods of this paper. It will be noted that agreement between the two values is remarkably good, particularly for the stronger bands which are of greatest importance in astrophysical applications. Agreement is adequate for weak bands, where the Franck-Condon factors $\sim 10^{-3}$ and there is strong cancellation. The q values for weak bands are seldom needed in applications. It is also noted that the array of "realistic" Franck-Condon factors is not symmetrical, that is $q(m, n) \neq q(n, m)$ because of the asymmetry of real potentials.

Sauval (1978), in his contribution to the meetings of Commission 14 of the IAU Montreal 1979 General Assembly, distributed a very useful list (Sauval 1979) of astrophysical molecules for which more spectroscopic data, particularly Franck-Condon factors and band oscillator strengths, were badly needed. Band systems of CeO, CoH, CrO, CuH, GeH, LaO, NiH, SnH, and ZnH were particularly emphasized in connection with S-type stars.

A critical review of the molecular data available for band systems of these molecules was made using the monograph of Huber and Herzberg (1979). The relevant ω_e , r_e , and μ_A data were then applied to the equations of Table 1 to calculate Franck-Condon factors for astrophysically important band systems of these molecules. Table 3 displays the molecular data which were used in these calculations. Tables 4-20 display the Franck-Condon factors, and band wavelengths calculated for

the $0 \leq v', v'' \leq 3$ array of bands of each of the 17 band systems involved. Band systems of CrH and Sn²H not specifically mentioned in Sauval's list are also included.

The estimated band wavelengths in Tables 4-20 are calculated from

$$\lambda(v', v'') = [\nu_{00} + \omega'_e(v' + 1/2) - \omega''_e(v'' + 1/2)]^{-1}, \quad (12)$$

appropriate to a simple harmonic oscillator model which is all that can be used if only ω'_e , ω''_e , and ν_{00} are available. The approximate location of each band is thereby specified. In the few cases where measured band head data are available (Suchert 1975; Rosen 1970; Pearse and Gaydon 1976), agreement with the location of observed bands is adequate to confirm identifications. In view of the approximations involved, no corrections have been applied to convert vacuum wavenumbers to air wavelengths. Band data are listed in order of increasing wavelength in the tables, on each of which specific S , t , and u values are also given.

While ω'_e , ω''_e , r'_e , r''_e , and μ_A were available for many of the states in Huber and Herzberg's (1979) compilation, in a few cases ω_e and/or r_e values were missing. Birge's rule, $\omega_e r_e^2 \sim \text{constant}$ for all electronic states of a molecule, was used in such cases to provide reasonable estimates of the missing data, indicated by footnotes in Table 3 for $r_e(A)$ of CoH, $r_e(B)$ and $\omega_e(A)$ of NiH, and $\omega_e(A)$ and $\omega_e(X)$ of Sn¹H. The ω_e and r_e data for Sn²H were used in estimations of ω_e data for Sn¹H.

The bands treated in Tables 4-20 lie in the 3500-10,500 Å wavelength range. The band systems fall in three regions of the parameter S ; viz., very small (0.07), small (0.2-0.5), medium (0.8-1.5). When S is very small, the $\Delta v=0$ sequence dominates the system, and $q(a, a) > 0.9$, $0 \leq a \leq 3$, as seen in the case of LaO($C-X$). The q

TABLE 3
MOLECULAR DATA USED IN THIS PAPER, EXTRACTED FROM THE COMPILATION OF HUBER AND HERZBERG (1979)

| Molecules | States | $\omega_e(\text{cm}^{-1})$ | $r_e(\text{\AA})$ | $\nu_{00}(\text{cm}^{-1})$ |
|--|--|---|---|---|
| AlO ($\mu_A = 10.0419$) | $B^2\Sigma$ $X^2\Sigma$ | 870.05 979.23 | 1.667 1.6179 | $B - X$: 20635.22 ... |
| CeO ($\mu_A = 14.35388$) | F_2 C_1 B_2 A_1 $X_2^3\Phi_3$ $X_1^3\Phi_3$ | 772 798 771 749 822.76 862 | 1.82426 1.83222 1.83958 1.8404 1.81175 1.82009 | $F_2 - X_2$: 20834.21 $C_1 - X_1$: 20273.84 $B_2 - X_2$: 13804.01 $A_1 - X_1$: 1295.75 |
| CoH ^a ($\mu_A = 0.99088$) | $A^3\Phi_4$ $X^3\Phi_4$ | 1527.8 1630.29 | 1.5394 ^a 1.5424 | $A - X$: 22243.4 ... |
| CrH ($\mu_A = 0.98864$) | $A^6\Sigma^+$ $X^6\Sigma^+$ | 1479.4 1581.2 | 1.787 1.6557 | $A - X$: 11552.29 ... |
| CrO ($\mu_A = 12.229027$) | $B^5\Pi$ $X^5\Pi$ | 750.5 898.4 | 1.703 1.615 | $B - X$: 16506.94 ... |
| CuH ($\mu_A = 0.99193979$) | $A^1\Sigma^+$ $X^1\Sigma^+$ | 1698.4 1941.26 | 1.5724 1.46263 | $A - X$: 23311.1 ... |
| GeH ($\mu_A = 0.993897979$) | $A^2\Delta$ $X^2\Pi_r$ | 1185.15 1833.77 | 1.611 1.588 | $A - X$: 25197 ... |
| LaO ($\mu_A = 14.343302$) | $C^2\Pi$ $B^2\Sigma^+$ $A^2\Pi$ $X^2\Sigma^+$ | 792.5 730.4 757.48 812.75 | 1.8295 1.8557 1.8422 1.8257 | $C - X$: 22729.24 $B - X$: 17837.8 $A - X$: 13066.64 ... |
| NiH ^b ($\mu_A = 0.9905931$) | $B^2\Delta$ $A^2\Delta$ $X^2\Delta$ | 1570.9 1548.726 ^b 1926.6 | 1.63414 ^b 1.6458 1.4756 | $B - X$: 15977.3 $A - X$: 15520.1 ... |
| Sn ¹ H ^c ($\mu_A = 0.999426$) | $A^2\Delta$ $X^2\Pi$ | 723.7 ^c 1182 ^c | 1.8546 1.78146 | $A - X$: 23468.27 ... |
| Sn ² H ^c ($\mu_A = 1.980828$) | $A^2\Delta$ $X^2\Delta$ | 736 1188 | 1.8391 1.777 | $A - X$: 23563.65 ... |
| ZnH ($\mu_A = 0.99218372$) | $A^2\Pi$ $X^2\Sigma$ | 1910.2 1607.6 | 1.5119 1.5947 | $A - X$: 23431.8 ... |

^aBirge's rule used to infer values of $r_e(A)$ of CoH (see text).

^bBirge's rule used to infer values of $r_e(B)$ and $\omega_e(A)$ of NiH (see text).

^cBirge's rule used to infer values of $\omega_e(A)$ and $\omega_e(X)$ of Sn¹H from data of Sn²H (see text).

values for other bands are negligible. When S is small, the $\Delta v = 0$ sequence still contains the strongest bands, and $q(0,0)$ is largest, but some contributions are made by the $\Delta v = \pm 1$ sequences. When $S \approx 1$ the $\Delta v = 0$ sequence is not as important as the $\Delta v = \pm 1, \pm 2$ sequences, and $q(0,0)$ is not the strongest band of the system. The Condon loci in these cases have widened. These observations are consistent with the graphs of Figures 1, 2, and 3.

For applications to the spectroscopy of cooler stellar envelopes, absorption transitions have to be considered. The $v'' = 0$ and $v'' = 1$ progressions are the most im-

portant. Which absorption bands of these progressions are strong, and where they lie can be inferred from Tables 4–20. The $q(v', v'')$ and $\lambda(v', v'')$ data of these tables are thus useful for identification purposes, as well as for diagnostic purposes and radiative transfer calculations.

As indicated in Tables 10, 13, and 14, alternative Franck-Condon factor data exist for the CrO($B - X$) and LaO($A - X$), LaO($b - X$) systems. The "Morse" calculations by Murthy and Nagaraj (1964) and by Ortenberg, Glasko, and Dmitriev (1964), respectively, use older and somewhat different molecular data.

TABLE 4
FRANCK-CONDON FACTORS FOR BANDS OF THE
CeO ($A_1-X_1^3\Phi_2$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 10012 | (0, 3) | 5.43-5 |
| 9313 | (1, 3) | 6.62-3 |
| 9225 | (0, 2) | 2.31-3 |
| 8706 | (2, 3) | 1.71-1 |
| 8629 | (1, 2) | 1.22-1 |
| 8553 | (0, 1) | 6.57-2 |
| 8173 | (3, 3) | 5.91-1 |
| 8105 | (2, 2) | 6.92-1 |
| 8308 | (1, 1) | 8.05-1 |
| 7972 | (0, 0) | 9.32-1 |
| 7641 | (3, 2) | 1.71-1 |
| 7581 | (2, 1) | 1.22-1 |
| 7523 | (1, 0) | 6.57-2 |
| 7174 | (3, 1) | 6.62-3 |
| 7121 | (2, 0) | 2.31-3 |
| 6761 | (3, 0) | 5.43-5 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.375$; $t=2.18$; $n=0.07$.

TABLE 5
FRANCK-CONDON FACTORS FOR BANDS OF THE
CeO ($B_2-X_2^3\Phi^3$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 8842 | (0, 3) | 3.31-4 |
| 8278 | (1, 3) | 2.07-2 |
| 8242 | (0, 2) | 7.55-3 |
| 7781 | (2, 3) | 2.62-1 |
| 7750 | (1, 2) | 2.01-1 |
| 7719 | (0, 1) | 1.15-1 |
| 7341 | (3, 3) | 3.50-1 |
| 7313 | (2, 2) | 4.88-1 |
| 7285 | (1, 1) | 6.61-1 |
| 7258 | (0, 0) | 8.77-1 |
| 6923 | (3, 2) | 2.62-1 |
| 6898 | (2, 1) | 2.01-1 |
| 6873 | (1, 0) | 1.15-1 |
| 6549 | (3, 1) | 2.07-3 |
| 6527 | (2, 0) | 7.55-3 |
| 6215 | (3, 0) | 3.31-4 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.512$, $t=2.98$, $u=0.131$.

TABLE 6
FRANCK-CONDON FACTORS FOR BANDS OF THE
CeO ($C_1-X_1^3\Phi_2$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5664 | (0, 3) | 2.81-6 |
| 5419 | (1, 3) | 9.62-4 |
| 5400 | (0, 2) | 3.26-4 |
| 5194 | (2, 3) | 7.18-2 |
| 5177 | (1, 2) | 4.81-2 |
| 5160 | (0, 1) | 2.52-1 |
| 4988 | (3, 3) | 8.31-1 |
| 4972 | (2, 2) | 8.77-1 |
| 4956 | (1, 1) | 9.25-1 |
| 4940 | (0, 0) | 9.74-1 |
| 4782 | (3, 2) | 7.18-2 |
| 4767 | (2, 1) | 4.91-2 |
| 4753 | (1, 0) | 2.52-1 |
| 4593 | (3, 1) | 9.62-4 |
| 4579 | (2, 0) | 3.26-4 |
| 4418 | (3, 0) | 2.81-6 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.228$, $t=1.32$, $u=0.026$.

TABLE 7
FRANCK-CONDON FACTORS FOR BANDS OF THE
CeO ($F_2-X_2^3\Phi_3$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5452 | (0, 3) | 3.03-6 |
| 5232 | (1, 3) | 1.01-3 |
| 5218 | (0, 2) | 3.43-4 |
| 5029 | (2, 3) | 7.35-2 |
| 5016 | (1, 2) | 5.03-2 |
| 5003 | (0, 1) | 2.58-2 |
| 4841 | (3, 3) | 8.27-1 |
| 4829 | (2, 2) | 8.74-1 |
| 4817 | (1, 1) | 9.23-1 |
| 4806 | (0, 0) | 9.74-1 |
| 4656 | (3, 2) | 7.35-2 |
| 4645 | (2, 1) | 5.03-2 |
| 4634 | (1, 0) | 2.58-2 |
| 4484 | (3, 1) | 1.01-3 |
| 4474 | (2, 0) | 3.43-4 |
| 4324 | (3, 0) | 3.03-6 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.23$, $t=1.34$, $u=0.026$.

TABLE 8
FRANCK-CONDON FACTORS FOR BANDS OF THE
CoH ($A^3\Phi_4-X^3\Phi_u$) SYSTEM^a

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^b |
|-------------------|-----------------------|---------------------------|
| 5780 | (0, 3) | 3.43-5 |
| 5311 | (1, 3) | 4.93-3 |
| 5282 | (0, 2) | 1.71-3 |
| 4912 | (2, 3) | 1.51-1 |
| 4888 | (1, 2) | 1.07-1 |
| 4863 | (0, 1) | 5.68-2 |
| 4569 | (3, 3) | 6.40-1 |
| 4548 | (2, 2) | 7.31-1 |
| 4527 | (1, 1) | 8.31-1 |
| 4506 | (0, 0) | 9.41-1 |
| 4253 | (3, 2) | 1.51-1 |
| 4234 | (2, 1) | 1.07-1 |
| 4216 | (1, 0) | 5.68-2 |
| 3977 | (3, 1) | 4.93-3 |
| 3961 | (2, 0) | 1.71-3 |
| 3735 | (3, 0) | 3.43-5 |

^aNote that Birge's rule was applied to estimate the value of $r_e(A)$.

^bThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.347$, $t=2.02$, $u=0.060$.

TABLE 10
FRANCK-CONDON FACTORS FOR BANDS OF THE
CrO ($B^5\Pi-X^5\Pi$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a | $q_M(v', v'')$ ^{a, b} |
|-------------------|-----------------------|---------------------------|--------------------------------|
| 9711 | (0, 3) | 8.03-2 | 6.9-2 |
| 9051 | (1, 3) | 2.39-1 | 2.94-1 |
| 8932 | (0, 2) | 2.09-1 | 2.23-1 |
| 8476 | (2, 3) | 5.35-3 | 4.0-3 |
| 8371 | (1, 2) | 2.39-1 | 1.49-1 |
| 8268 | (0, 1) | 3.64-1 | 3.98-1 |
| 7969 | (3, 3) | 1.64-1 | 1.44-1 |
| 7876 | (2, 2) | 1.29-1 | 1.49-1 |
| 7785 | (1, 1) | 7.18-3 | 1.6-2 |
| 7697 | (0, 0) | 3.16-1 | 2.95-1 |
| 7437 | (3, 2) | 5.35-3 | 6.0-3 |
| 7355 | (2, 1) | 2.39-1 | 6.0-2 |
| 7276 | (1, 0) | 3.64-1 | 3.11-1 |
| 6971 | (3, 1) | 2.39-1 | 1.48-1 |
| 6900 | (2, 0) | 2.09-1 | 2.0-1 |
| 6560 | (3, 0) | 8.03-2 | 1.05-1 |

^aThe negative number is the power of 10 by which the entry is multiplied.

^b"Morse" Franck-Condon factors of Murthy and Nagaraj (1964) based on somewhat different molecular constants.

NOTE.— $S=1.52$, $t=8.81$, $u=1.155$.

TABLE 9
FRANCK-CONDON FACTORS FOR BANDS OF THE
CrH ($A^6\Sigma^+-X^6\Sigma^+$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 14798 | (0, 3) | 6.53-3 |
| 12140 | (1, 3) | 1.16-1 |
| 11992 | (0, 2) | 5.07-2 |
| 10292 | (2, 3) | 3.21-1 |
| 10080 | (0, 1) | 2.63-1 |
| 8932 | (3, 3) | 2.06-3 |
| 8851 | (2, 2) | 6.19-2 |
| 8772 | (1, 1) | 2.56-1 |
| 8695 | (0, 0) | 6.79-1 |
| 7826 | (3, 2) | 3.21-1 |
| 7765 | (2, 1) | 3.42-1 |
| 6964 | (3, 1) | 1.16-1 |
| 6916 | (2, 0) | 5.07-2 |
| 6274 | (3, 0) | 6.53-3 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.880$, $t=5.10$, $u=0.387$.

TABLE 11
FRANCK-CONDON FACTORS FOR BANDS OF THE
CuH ($A^1\Sigma^+-X^1\Sigma^+$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5758 | (0, 3) | 4.01-3 |
| 5245 | (1, 3) | 8.96-2 |
| 5179 | (0, 2) | 3.75-2 |
| 4816 | (2, 3) | 3.39-1 |
| 4761 | (1, 2) | 3.28-1 |
| 4706 | (0, 1) | 2.33-1 |
| 4452 | (3, 3) | 2.49-2 |
| 4405 | (2, 2) | 1.21-2 |
| 4358 | (1, 1) | 3.34-1 |
| 4313 | (0, 0) | 7.25-1 |
| 4098 | (3, 2) | 3.39-1 |
| 4058 | (2, 1) | 3.28-1 |
| 4018 | (1, 0) | 2.33-1 |
| 3796 | (3, 1) | 8.96-2 |
| 3761 | (2, 0) | 3.75-2 |
| 3535 | (3, 0) | 4.01-3 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.818$, $t=4.66$, $u=0.335$.

TABLE 12
FRANCK-CONDON FACTORS FOR BANDS OF THE
GeH ($A^2\Delta-X^2\Pi$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5162 | (0, 3) | 2.41-7 |
| 4865 | (1, 3) | 1.90-4 |
| 4716 | (0, 2) | 6.38-5 |
| 4599 | (2, 3) | 3.29-2 |
| 4466 | (1, 2) | 2.22-2 |
| 4362 | (3, 3) | 9.23-1 |
| 4340 | (0, 1) | 1.22-2 |
| 4242 | (2, 2) | 9.44-1 |
| 4128 | (1, 1) | 9.66-1 |
| 4039 | (3, 2) | 3.29-2 |
| 4020 | (0, 0) | 9.89-1 |
| 3936 | (2, 1) | 2.22-2 |
| 3838 | (1, 0) | 1.22-2 |
| 3760 | (3, 1) | 1.90-4 |
| 3671 | (2, 0) | 6.38-5 |
| 3518 | (3, 0) | 2.41-7 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.151$, $t=0.875$, $u=0.011$.

TABLE 13
FRANCK-CONDON FACTORS FOR BANDS OF THE
LaO ($A^2\Pi-X^2\Sigma^+$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a | $q_M(v', v'')$ ^{a, b} |
|-------------------|-----------------------|---------------------------|--------------------------------|
| 9433 | (0, 3) | 1.49-5 | 2.0-5 |
| 8804 | (1, 3) | 2.87-3 | 4.27-3 |
| 8762 | (0, 2) | 9.86-4 | 1.45-3 |
| 8254 | (2, 3) | 1.19-1 | 1.0-1 |
| 8216 | (1, 2) | 8.29-2 | 6.99-2 |
| 8179 | (0, 1) | 4.34-2 | 3.64-2 |
| 7768 | (3, 3) | 7.18-1 | 7.46-1 |
| 7735 | (2, 2) | 7.92-1 | 8.16-1 |
| 7702 | (1, 1) | 8.71-1 | 8.88-1 |
| 7669 | (0, 0) | 9.56-1 | 9.62-1 |
| 7307 | (3, 2) | 1.19-1 | 1.10-1 |
| 7277 | (2, 1) | 8.29-2 | 7.45-2 |
| 7248 | (1, 0) | 4.34-2 | 3.76-2 |
| 6897 | (3, 1) | 2.87-3 | 9.4-4 |
| 6871 | (2, 0) | 9.86-4 | 2.7-4 |
| 6531 | (3, 0) | 1.49-5 | 1.0-5 |

^aThe negative number is the power of 10 by which the entry is multiplied.

^b“Morse” Franck-Condon factors of Ortenberg, Glasko, and Dmitriev (1964) based on somewhat different molecular constants.

NOTE.— $S=0.301$, $t=1.75$, $u=0.045$.

TABLE 14
FRANCK-CONDON FACTORS FOR BANDS OF THE
LaO ($B^2\Sigma^+-X^2\Sigma^+$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a | $q_M(v', v'')$ ^{a, b} |
|-------------------|-----------------------|---------------------------|--------------------------------|
| 6511 | (0, 3) | 4.60-4 | 9.2-4 |
| 6216 | (1, 3) | 2.54-2 | 3.57-2 |
| 6184 | (0, 2) | 9.37-3 | 1.34-2 |
| 5946 | (2, 3) | 2.80-1 | 2.32-1 |
| 5917 | (1, 2) | 2.18-1 | 2.04-1 |
| 5888 | (0, 1) | 1.27-1 | 1.23-1 |
| 5698 | (3, 3) | 3.00-1 | 2.93-1 |
| 5672 | (2, 2) | 4.43-1 | 4.37-1 |
| 5645 | (1, 1) | 6.27-1 | 6.26-1 |
| 5619 | (0, 0) | 8.63-1 | 8.63-1 |
| 5446 | (3, 2) | 2.80-1 | 3.06-1 |
| 5422 | (2, 1) | 2.18-1 | 2.32-1 |
| 5398 | (1, 0) | 1.27-1 | 1.30-1 |
| 5215 | (3, 1) | 2.54-2 | 1.94-2 |
| 5193 | (2, 0) | 9.37-3 | 6.54-3 |
| 5003 | (3, 0) | 4.60-4 | 3.0-5 |

^aThe negative number is the power of 10 by which the entry is multiplied.

^b“Morse” Franck-Condon factors of Ortenberg, Glasko, and Dmitriev (1964) based on somewhat different molecular constants.

NOTE.— $S=0.543$, $t=3.15$, $u=0.147$.

TABLE 15
FRANCK-CONDON FACTORS FOR BANDS OF THE
LaO ($C^2\Pi_r-X^2\Sigma^+$) SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 4931 | (0, 3) | 2.50-9 |
| 4745 | (1, 3) | 9.07-6 |
| 4741 | (0, 2) | 3.03-6 |
| 4573 | (2, 3) | 7.34-3 |
| 4569 | (1, 2) | 4.90-3 |
| 4565 | (0, 1) | 2.46-3 |
| 4413 | (3, 3) | 9.83-1 |
| 4409 | (2, 2) | 9.88-1 |
| 4406 | (1, 1) | 9.93-1 |
| 4402 | (0, 0) | 9.98-1 |
| 4261 | (3, 2) | 7.34-3 |
| 4257 | (2, 1) | 4.90-3 |
| 4253 | (1, 0) | 2.46-3 |
| 4118 | (3, 1) | 9.07-6 |
| 4115 | (2, 0) | 3.03-6 |
| 3985 | (3, 0) | 2.50-9 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.07$, $t=0.408$, $u=2.45-3^a$.

TABLE 16
FRANCK-CONDON FACTORS FOR BANDS OF THE
NiH ($A^2\Delta-X^2\Delta$) SYSTEM^a

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^b |
|-------------------|-----------------------|---------------------------|
| 10470 | (0, 3) | 3.15-2 |
| 9009 | (1, 3) | 2.21-1 |
| 8712 | (0, 2) | 1.29-1 |
| 7906 | (2, 3) | 1.34-1 |
| 7677 | (1, 2) | 2.83-1 |
| 7460 | (0, 1) | 3.52-1 |
| 7043 | (3, 3) | 1.01-1 |
| 6861 | (2, 2) | 1.87-2 |
| 6687 | (1, 1) | 3.43-2 |
| 6523 | (0, 0) | 4.81-1 |
| 6202 | (3, 2) | 1.34-1 |
| 6060 | (2, 1) | 2.83-1 |
| 5924 | (1, 0) | 3.52-1 |
| 5540 | (3, 1) | 2.21-1 |
| 5426 | (2, 0) | 1.29-1 |
| 5006 | (3, 0) | 3.15-2 |

^aNote that Birge's rule was used to estimate the value of $\omega_e(A)$.
^bThe negative number is the power of 10 by which the entry is multiplied.
NOTE.— $S=1.21$, $t=7.03$, $u=0.732$.

TABLE 18
FRANCK-CONDON FACTORS FOR BANDS OF THE
Sn¹H ($A^2\Delta-X^2\Pi$) SYSTEM^a

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5078 | (0, 3) | 5.84-5 |
| 4898 | (1, 3) | 6.93-3 |
| 4790 | (0, 2) | 2.43-3 |
| 4730 | (2, 3) | 1.74-1 |
| 4630 | (1, 2) | 1.25-1 |
| 4574 | (3, 3) | 5.82-1 |
| 4534 | (0, 1) | 6.72-2 |
| 4480 | (2, 2) | 6.85-1 |
| 4390 | (1, 1) | 8.01-1 |
| 4339 | (3, 2) | 1.74-1 |
| 4303 | (0, 0) | 9.30-1 |
| 4255 | (2, 1) | 1.25-1 |
| 4173 | (1, 0) | 6.72-2 |
| 4127 | (3, 1) | 6.93-3 |
| 4051 | (2, 0) | 2.43-3 |
| 3935 | (3, 0) | 5.84-5 |

^aNote that Birge's rule and the molecular constants of Sn²H (see Table 3) were used to estimate values of $\omega_e(A)$, $\omega_e(X)$ of Sn¹H.
^bThe negative number is the power of 10 by which the entry is multiplied.
NOTE.— $S=0.38$, $t=2.21$, $u=0.072$.

TABLE 17
FRANCK-CONDON FACTORS FOR BANDS OF THE
NiH ($B^2\Delta-X^2\Delta$) SYSTEM^a

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^b |
|-------------------|-----------------------|---------------------------|
| 5723 | (0, 3) | 2.31-2 |
| 5251 | (1, 3) | 2.01-1 |
| 5154 | (0, 2) | 1.08-1 |
| 4851 | (2, 3) | 1.85-1 |
| 4768 | (1, 2) | 3.12-1 |
| 4689 | (0, 1) | 3.38-1 |
| 4507 | (3, 3) | 6.46-1 |
| 4436 | (2, 2) | 3.04-3 |
| 4367 | (1, 1) | 6.81-2 |
| 4300 | (0, 0) | 5.27-1 |
| 4147 | (3, 2) | 1.85-1 |
| 4087 | (2, 1) | 3.12-1 |
| 4028 | (1, 0) | 3.38-1 |
| 3840 | (3, 1) | 2.01-1 |
| 3788 | (2, 0) | 1.08-1 |
| 3576 | (3, 0) | 2.31-2 |

^aNote that Birge's rule was used to estimate the value of $r_e(B)$.
^bThe negative number is the power of 10 by which the entry is multiplied.
NOTE.— $S=1.13$, $t=6.57$, $u=0.638$.

TABLE 19
FRANCK-CONDON FACTORS FOR BANDS OF THE
Sn²H ($A^2\Delta-X^2\Delta$) SYSTEM^a

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^b |
|-------------------|-----------------------|---------------------------|
| 5057 | (0, 3) | 1.71-4 |
| 4876 | (1, 3) | 1.37-3 |
| 4771 | (0, 2) | 4.91-3 |
| 4707 | (2, 3) | 2.27-1 |
| 4609 | (1, 2) | 1.69-1 |
| 4549 | (3, 3) | 4.45-1 |
| 4515 | (0, 1) | 9.41-2 |
| 4458 | (2, 2) | 5.72-1 |
| 4370 | (1, 1) | 7.23-1 |
| 4316 | (3, 2) | 2.27-1 |
| 4285 | (0, 0) | 9.01-1 |
| 4233 | (2, 1) | 1.69-1 |
| 4154 | (1, 0) | 9.41-2 |
| 4105 | (3, 1) | 1.37-2 |
| 4031 | (2, 0) | 4.91-3 |
| 3915 | (3, 0) | 1.71-4 |

^aNote that molecular constants of this system were used by application of Birge's rule to estimate $\omega_e(A)$ and $r_e(B)$ of Sn¹H (see Tables 3 and 18).
^bThe negative number is the power of 10 by which the entry is multiplied.
NOTE.— $S=0.457$, $t=2.65$, $u=0.104$.

TABLE 20
FRANCK-CONDON FACTORS FOR BANDS
OF THE $\text{ZnH } (A^2\Pi - X^2\Sigma)$ SYSTEM

| Wavelength (Å) | Band (v', v'') | $q(v', v'')$ ^a |
|-------------------|-----------------------|---------------------------|
| 5330 | (0, 3) | 7.67-4 |
| 4910 | (0, 2) | 1.30-2 |
| 4838 | (1, 3) | 3.47-2 |
| 4551 | (0, 1) | 1.48-1 |
| 4489 | (1, 2) | 2.46-1 |
| 4429 | (2, 3) | 3.05-1 |
| 4240 | (0, 0) | 8.38-1 |
| 4187 | (1, 1) | 2.24-1 |
| 4134 | (2, 3) | 3.68-1 |
| 4083 | (3, 3) | 2.24-1 |
| 3923 | (1, 0) | 1.48-1 |
| 3877 | (2, 1) | 2.46-1 |
| 3832 | (3, 2) | 3.05-1 |
| 3649 | (2, 0) | 1.30-2 |
| 3609 | (3, 1) | 3.47-2 |
| 3411 | (3, 0) | 7.67-4 |

^aThe negative number is the power of 10 by which the entry is multiplied.

NOTE.— $S=0.594$, $t=3.45$, $u=0.176$.

Nevertheless, quite good agreement in general exists between their data and those of this paper, except for the very weak bands.

IV. CONCLUSIONS

The simple expressions of Table 1 can be used with confidence to estimate Franck-Condon factors of low vibrational quantum number bands of systems for which ω_e , r_e , and μ_A values are known, such as is often the case for astrophysically important molecules.

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R. W. NICHOLLS: Center for Research in Experimental Space Science, York University, 4700 Keele St., Downsview, Ontario M3J 1P3, Canada