

Franck-Condon Factors to High Vibrational Quantum Numbers V: O₂ Band Systems

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Franck-Condon factors arrays have been computed numerically and are displayed to highest known vibrational quantum numbers for the following O₂ band systems:

Herzberg I:	(A ³ Σ _u ⁺ – X ³ Σ _g [–])
Herzberg II:	(c ¹ Σ _u [–] – X ³ Σ _g [–])
Herzberg III:	(D ³ Δ _u – X ³ Σ _g [–])
Chamberlain:	(D ³ Δ _u – a ¹ Δ _g)
Broida-Gaydon:	(A ³ Σ _u ⁺ – b ¹ Σ _g ⁺)
Noxon:	(b ¹ Σ _g ⁺ – a ¹ Δ _g)
Atmospheric	(b ¹ Σ _g ⁺ – X ³ Σ _g [–])
Infrared Atmospheric:	(a ¹ Δ _g – X ³ Σ _g [–])

1. Introduction

The most important band systems of O₂, most of which have applications in aeronomy, are listed in table 1 with descriptive comments. They are also indicated in the simplified energy level diagram (figure 1). They cover the broad spectral region from the vacuum ultraviolet to the near infrared. Most of them are hard to excite in emission in simple discharges for one of two reasons. Either excitation from the ground state to the upper state concerned results in dissociation because of the relative position of the potentials, and the operation of the Franck-Condon principle (e.g., Schumann-Runge and Herzberg I systems) or even if the bound upper state can be excited from the ground state, the emission transitions from the upper state are often forbidden for dipole radiation (e.g., Herzberg II, Chamberlain, Broida-Gaydon, Atmospheric and Infrared Atmospheric), and the excited molecules are depopulated by collisions with other molecules or the walls before they can radiate. Special light sources have therefore been developed for emission studies [Feast, 1949, Broida and Gaydon 1954, Broida and Peyron 1960, Barth and Patapoff, 1962]. Further, the preponderance of forbidden transitions involving the ground state indicates the need for long path lengths and exposure times for absorption studies. [Herzberg and Herzberg, 1947, Babcock and Herzberg 1948, Ditchburn and Heddle, 1954, Ditchburn and Young, 1962]. The band systems are well documented in the compilations of Wallace [1962] and of Pearse and Gaydon [1963].

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TABLE 1. Band systems of O₂

Band system	Wavelength range (Å)	Reference
Schumann-Runge (B ³ Σ _u [–] – X ³ Σ _g [–])	1751–5720	[1]
Herzberg I (A ³ Σ _u ⁺ – X ³ Σ _g [–])	2429–4881	[2]
Herzberg II (c ¹ Σ _u [–] – X ³ Σ _g [–])	2540–6541	[3]
Herzberg III (D ³ Δ _u – X ³ Σ _g [–])	2570–2630	[3]
Broida-Gaydon (A ³ Σ _u ⁺ – b ¹ Σ _g ⁺)	3596–5631	[4]
Chamberlain (D ³ Δ _u – a ¹ Δ _g)	3696–4379	[5]
Atmospheric (b ¹ Σ _g ⁺ – X ³ Σ _g [–])	5795–8645	[6]
Infrared atmospheric (a ¹ Δ _g – X ³ Σ _g [–])	10, 600–15, 800	[7]
Noxon (b ¹ Σ _g ⁺ – a ¹ Δ _g)	19, 100	[8]

References:

- [1] Feast (1949).
- [2] Herzberg (1952).
- [3] Herzberg (1953).
- [4] Broida and Gaydon (1954).
- [5] Chamberlain (1958).
- [6] Babcock and Herzberg (1948).
- [7] Herzberg and Herzberg (1947).
- [8] Noxon (1961).

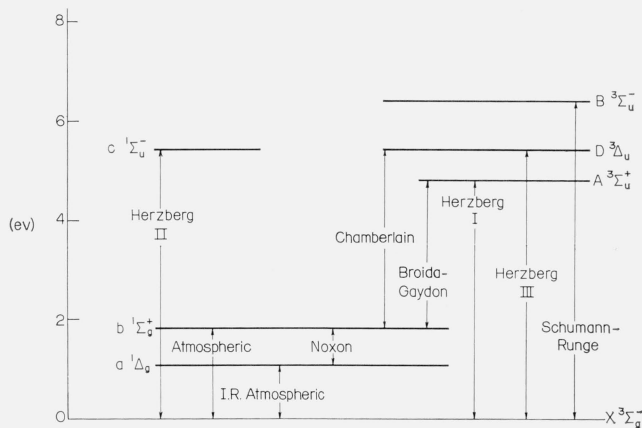


FIGURE 1. Partial energy level diagram for O_2 .

The band strength $S_{v'v''}$, defined in eq (1) in terms of Franck-Condon factor $q_{v'v''}$ and the electronic transition moment $R_e(\bar{r}_{v'v''})$ determines, apart from powers of frequency, such important transition probability parameters as band absorption coefficient $k_{v'v''}$, band oscillator strength $f_{v'v''}$, band Einstein A and B coefficients $A_{v'v''}$, $B_{v'v''}$ and integrated emission intensity of the band $I_{v'v''}$, as indicated in eqs (2a-e). $\bar{r}_{v'v''}$ is the r -centroid of the band.

$$S_{v'v''} = R_e^2(\bar{r}_{v'v''}) q_{v'v''} \quad (1)$$

$$B_{v'v''} \propto S_{v'v''} \quad (2a)$$

$$k_{v'v''} \propto \nu_{v'v''} S_{v'v''} \quad (2b)$$

$$f_{v'v''} \propto \nu_{v'v''} S_{v'v''} \quad (2c)$$

$$A_{v'v''} \propto \nu_{v'v''}^3 S_{v'v''} \quad (2d)$$

$$I_{v'v''} \propto \nu_{v'v''}^4 S_{v'v''} \quad (2e)$$

Thus, as is well known, and has been pointed out in earlier papers of this series [Nicholls, 1961], the Franck-Condon factors exert a proportional and dominating influence on the transition probability parameters and intensity distributions within a band system.

It is the purpose of this paper, which is one of a series treating astrophysically and aeronomically important band systems, to present tables of Franck-Condon factors to high quantum numbers for all the band systems of O_2 listed in table 1 except for the Schumann-Runge system, which has been treated previously [Nicholls, 1960].

2. Method

The straightforward method of computer-based calculation described in the first paper of the series [Nicholls, 1961] was used and the calculations were performed in the computation center of the National

Bureau of Standards. Input data are ω_e , $\omega_e x_e$, r_e , and v_{\max} for each of the electronic states involved, and μ_A for the molecular species in question. The notation is conventional [Herzberg, 1950]. The Morse model of molecular potentials is adopted and the computer program provides all needed Morse vibrational wavefunctions and their overlap integral squares, the Franck-Condon factors. The Morse potential is admittedly an empirical expedient, but for many of the systems treated here the range of vibrational quantum numbers involved is sufficiently small that it is probably realistic. Further, in many cases, the molecular constants needed for evaluation of a more realistic potential are not available (see sec. 4, discussion).

The input data employed in the calculations are summarized with references in table 2. These data were obtained from original papers with the exception of the $D^3\Delta_u$ and $A^3\Sigma_u^+$ states. Constants for

TABLE 2. Basic data

State	$\omega_e(\text{cm}^{-1})$	$\omega_e x_e(\text{cm}^{-1})$	$r_e(\text{\AA})$	v_{\max}	Reference
$X^3\Sigma_g^-$	1580.3613	12.073	1.207398	12	[1]
$A^3\Sigma_u^+$	802.795	14.635	1.514	12	[2, 3]
$D^3\Delta_u$	791	15	1.4802	6	[3, 4, 5]
$a^1\Delta_g$	1509.03	12.9	1.2155	5	[1]
$b^1\Sigma_g^+$	1432.687	13.95	1.22675	3	[1]
$c^1\Sigma_u^+$	650.49	17.036	1.597	6	[4]

$\mu_A = 8.0000$ for all states

References:

- [1] Herzberg (1950).
- [2] Herzberg (1952).
- [3] See comments in text.
- [4] Herzberg (1953).
- [5] Chamberlain (1958).

the $D^3\Delta_u$ state were computed as follows: Herzberg's [1953] absorption measurements on the $v''=0$, $v'=6$ and $v''=0$, $v'=5$ bands provided B_v values for the $v'=5$ and 6 levels from which $\alpha_e=0.0262 \text{ cm}^{-1}$, $B_e=0.9618 \text{ cm}^{-1}$, and $r_e=1.4802 \text{ \AA}$ were derived. Chamberlain's [1958] measured values of $\Delta G(5\frac{1}{2})$, $\Delta G(4\frac{1}{2})$, $\Delta G(3\frac{1}{2})$ led to the values of $\omega_e=791 \text{ cm}^{-1}$, $\omega_e x_e=15 \text{ cm}^{-1}$. Broida and Gaydon [1954] showed from emission measurements on the Herzberg I system that the vibrational numbering of the $A^3\Sigma_u^+$ state should be raised one unit above the values proposed by Herzberg [1952] from absorption studies. New ω_e , $\omega_e x_e$, and r_e values were therefore calculated for this state.

3. Results

Franck-Condon factor arrays are displayed in tables 3 through 10 for the band systems listed in table 1 with the exception of the Schumann-Runge system. The Condon loci [Nicholls, 1963; Murty, 1964] are indicated on the tables by setting entries for bands which lie on the local maxima of the Franck-Condon factor surfaces in bold-faced type. The large change in r_e which is associated with the

Herzberg I, II, III, Chamberlain and Broida-Gaydon systems, and which as was pointed out in the introduction makes them difficult to excite in conventional discharges, results in broad Condon loci well removed from (0, 0). The negative number in each entry is the power of ten by which it is multiplied.

4. Discussion

The Condon loci of tables 3 through 10 agree well with the $v'-v''$ positions of the commonly excited bands of each system [Pearse and Gaydon, 1963; Wallace, 1962].

TABLE 3. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Herzberg I ($A^3\Sigma_u^+ - X^3\Sigma_g^+$) band system*

$v' \backslash v''$	0	1	2	3	4	5	6	7	8	9	10	11	12
0	2.4260-6	4.4311-5	3.8195-4	2.0682-3	7.9015-3	2.2677-2	5.0829-2	9.1339-2	1.3404-1	1.6280-1	1.6531-1	1.4116-1	1.0235-1
1	1.7963-5	2.8498-4	2.0854-3	9.3083-3	2.8188-2	6.0734-2	9.4368-2	1.0346-1	7.3138-2	2.3803-2	1.2404-5	2.7251-2	8.5565-2
2	7.1157-5	9.8205-4	6.0930-3	2.2262-2	5.2426-2	8.0955-2	7.7534-2	3.6282-2	1.2808-3	1.8045-2	6.4243-2	7.4034-2	3.3088-2
3	2.0058-4	2.4117-3	1.2665-2	3.7533-2	6.6886-2	6.8355-2	3.0189-2	1.6908-4	2.3655-2	5.8664-2	4.0520-2	2.3991-3	1.8152-2
4	4.5158-4	4.7377-3	2.1011-2	4.9907-2	6.4623-2	3.7362-2	1.8959-3	1.6340-2	4.9053-2	3.0215-2	1.0245-4	2.6875-2	5.3812-2
5	8.6424-4	7.9236-3	2.9593-2	5.5466-2	4.8946-2	1.0699-2	5.0153-3	3.8195-2	3.2349-2	8.4136-4	2.1383-2	4.3836-2	1.1637-2
6	1.4615-3	1.1729-2	3.6766-2	5.3252-2	2.8664-2	1.7439-4	2.1532-2	3.6878-2	6.4788-3	1.0003-2	3.7852-2	1.3644-2	4.6200-3
7	2.2417-3	1.5774-2	4.1336-2	4.4970-2	1.1800-2	3.9240-3	3.2060-2	1.9645-2	6.5648-4	2.8007-2	2.1810-2	3.3556-4	2.8760-2
8	3.1772-3	1.9640-2	4.2823-2	3.3623-2	2.2931-3	1.3620-2	3.0297-2	4.4361-3	1.1216-2	2.8646-2	2.9320-3	1.4582-2	2.8214-2
9	4.2188-3	2.2959-2	4.1422-2	2.2133-2	4.5604-5	2.1779-2	2.0519-2	4.6861-5	2.1899-2	1.5626-2	1.5959-3	2.5866-2	9.2906-3
10	5.3038-3	2.5470-2	3.7782-2	1.2527-2	2.6733-3	2.4903-2	9.7307-3	4.4418-3	2.3701-2	3.5597-3	1.1442-2	2.0832-2	1.2637-5
11	6.3645-3	2.7042-2	3.2741-2	5.7337-3	7.3200-3	2.3080-2	2.5272-3	1.1446-2	1.7762-2	3.7198-5	1.9092-2	8.6868-3	5.4809-3
12	7.3364-3	2.7662-2	2.7108-2	1.7830-3	1.1771-2	1.8219-2	2.6400-5	1.6299-2	9.4564-3	3.5418-3	1.8912-2	9.3510-4	1.4294-2

TABLE 4. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Herzberg II ($c^1\Sigma_u^- - X^3\Sigma_g^-$) band system*

$v' \backslash v''$	0	1	2	3	4	5	6
0	4.9034-9	1.4332-7	1.9938-6	1.7584-5	1.1051-4	5.2734-4	1.9884-3
1	4.1810-8	1.1242-6	1.4242-5	1.1301-4	6.2969-4	2.6165-3	8.3984-3
2	1.8850-7	4.6808-6	5.4202-5	3.8821-4	1.9220-3	6.9550-3	1.8931-2
3	5.9754-7	1.3757-5	1.4616-4	9.4806-4	4.1804-3	1.3174-2	3.0257-2
4	1.4943-6	3.2023-5	3.1340-4	1.8477-3	7.2739-3	1.9960-2	3.8429-2
5	3.1363-6	6.2815-5	5.6860-4	3.0584-3	1.0779-2	2.5749-2	4.1214-2
6	5.7386-6	1.0787-4	9.0699-4	4.4689-3	1.4143-2	2.9405-2	3.8721-2

TABLE 5. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Herzberg III ($D^3\Delta_u - X^3\Sigma_g^-$) band system*

$v' \backslash v''$	0	1	2	3	4	5	6
0	3.8288-5	5.0005-4	3.0975-3	1.2120-2	3.3656-2	7.0662-2	1.1668-1
1	2.4088-4	2.6265-3	1.3122-2	3.9516-2	7.9017-2	1.0789-1	9.7341-2
2	8.1643-4	7.4212-3	2.9636-2	6.0945-2	9.0174-2	6.6456-2	1.6013-2
3	1.9828-3	1.4969-2	4.7330-2	7.7256-2	6.1957-2	1.3511-2	4.8898-3
4	3.8726-3	2.4327-2	5.9784-2	6.6592-2	2.3978-2	8.7565-4	3.6053-2
5	6.4728-3	3.3690-2	6.3271-2	4.3737-2	2.3910-3	1.8602-2	4.5742-2
6	9.6233-3	4.1397-2	5.7949-2	2.0779-2	2.0654-3	3.5565-2	2.7272-2

TABLE 6. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Broida-Gaydon ($A^3\Sigma_u^+ - b^1\Sigma_g^+$) band system*

$v' \backslash v''$	0	1	2	3
0	2.2109-5	3.5654-4	2.6485-3	1.2032-2
1	1.3876-4	1.8674-3	1.1145-2	3.8577-2
2	4.7218-4	5.3114-3	2.5349-2	6.5513-2
3	1.1574-3	1.0895-2	4.1317-2	7.7474-2
4	2.2911-3	1.8065-2	5.3976-2	7.0328-2
5	3.8947-3	2.5742-2	5.9911-2	5.0652-2
6	5.9050-3	3.2733-2	5.8463-2	2.8507-2
7	8.1905-3	3.8092-2	5.1199-2	1.1380-2
8	1.0582-2	4.1304-2	4.0705-2	2.1548-3
9	1.2903-2	4.2286-2	2.9494-2	4.6145-5
10	1.4998-2	4.1288-2	1.9398-2	2.5264-3
11	1.6748-2	3.8752-2	1.1403-2	6.9176-3
12	1.8074-2	3.5182-2	5.7788-3	1.1230-2

TABLE 7. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Chamberlain ($D^3\Delta_u - a^1\Delta_g$) band system*

$v' \backslash v''$	0	1	2	3	4	5
0	8.8377-5	1.0910-3	6.3151-3	2.2808-2	5.7690-2	1.0874-1
1	5.1497-4	5.1932-3	2.3502-2	6.2355-2	1.0543-1	1.1336-1
2	1.6268-3	1.3371-2	4.6693-2	8.7441-2	8.7958-2	3.5630-2
3	3.7032-3	2.4739-2	6.5508-2	8.1288-2	3.7238-2	5.2831-6
4	6.8150-3	3.6873-2	7.2326-2	5.3304-2	4.0037-3	1.9620-2
5	1.0785-2	4.7068-2	6.6223-2	2.3231-2	2.8569-3	4.2661-2
6	1.5248-2	5.3428-2	5.1505-2	4.6199-3	1.8481-2	4.1175-2

TABLE 8. *Franck-Condon factors to high vibrational quantum numbers for the O₂ Atmospheric (b¹Σ_g⁺—X³Σ_g⁻) band system*

$\begin{smallmatrix} v'' \\ v' \end{smallmatrix}$	0	1	2	3	4	5	6
0	9.3000-1	6.7294-2	2.6512-3	6.4085-5	9.3835-7	1.0341-8	3.7300-11
1	6.7276-2	7.8980-1	1.3396-1	8.6731-3	3.0158-4	5.9637-6	8.2523-8
2	2.6569-3	1.3360-1	6.4718-1	1.9695-1	1.8736-2	8.8087-4	2.2592-5
3	6.8742-5	8.9509-3	1.9530-1	5.0723-1	2.5298-1	3.3379-2	2.0431-3

TABLE 9. *Franck-Condon factors to high vibrational quantum numbers for the O₂ I-R Atmospheric (a¹Δ_g—X³Σ_g⁻) band system*

$\begin{smallmatrix} v'' \\ v' \end{smallmatrix}$	0	1	2	3	4	5	6
0	9.8692-1	1.2948-2	1.3605-4	2.4677-7	9.9011-10	1.5322-13	4.7034-13
1	1.3020-2	9.5876-1	2.7782-2	4.5133-4	1.2592-6	5.6454-9	1.1942-12
2	6.0566-5	2.8065-2	9.2637-1	4.4518-2	9.9828-4	3.9704-6	1.9449-8
3	6.0739-8	2.3808-4	4.5114-2	8.8969-1	6.3136-2	1.8396-3	9.9212-6
4	4.5740-8	3.5056-8	6.0928-4	6.4087-2	8.4869-1	8.3571-2	3.0493-3
5	2.2138-9	2.1350-7	6.0165-8	1.2732-3	8.4834-2	8.0346-1	1.0571-1

TABLE 10. *Franck-Condon factors to high vibrational quantum numbers for the Noxon (b¹Σ_g⁺—a¹Δ_g) band system*

$\begin{smallmatrix} v'' \\ v' \end{smallmatrix}$	0	1	2	3	4	5
0	9.7645-1	2.3320-2	2.3477-4	1.2155-6	7.7672-11	9.1536-11
1	2.3178-2	9.2694-1	4.9091-2	7.9620-4	5.7591-6	1.3075-9
2	3.6962-4	4.8450-2	8.7223-1	7.7152-2	1.7953-3	1.7072-5
3	5.0908-6	1.2698-3	7.5485-2	8.1260-1	1.0726-1	3.3637-3

Many of the band systems are important contributors to the spectrum of the airglow [Chamberlain, 1961]. Some $q_{v'v''}$ -values on primary Condon loci were therefore included in a compilation [Nicholls, 1964a] of transition probability data of aeronautical importance presented at the symposium on Laboratory Studies on Aeronomy held by the International Association for Geomagnetism and Aeronomy, Berkeley, August 1963. Similar treatment was given to some of the data of the previous paper of this series [Nicholls, 1964b] which deals with NO band systems.

The sum rule

$$\sum_{v' \text{ or } v''} q_{v'v''} + \int_{\text{Continuum}} dq_{v'v''} = 1 \quad (3)$$

appears to be satisfied by the contributions from the discrete bands for the Atmospheric, Infrared Atmospheric, and Noxon systems. However, in the case of the Herzberg I, II, III, Chamberlain and Broida-Gaydon systems, the contribution from the discrete bands is small, and a significant contribution can be expected from the photo-dissociation continuum, for, as was pointed out in section 1, dissociation is the most probable result of an upward transition in these cases according to the Franck-Condon principle. Studies have recently been made on the contribution of the Franck-Condon "density" in the

continuum for the Schumann-Runge system [Jarman and Nicholls, 1964] where it was found, for example, that 99.7 percent of the sum from $v'=0$ is in fact vested in the continuum. Realistic Klien-Dunham potentials were used and the work is currently being extended to the Herzberg I system.

One common criticism of Morse Franck-Condon factors is that they may be unrealistic for band systems for which the Morse potentials are not appropriate. The B³Σ_u⁻ upper state of the Schumann-Runge system is an example of such a case [Jarman, 1963a, b; Nicholls and Jarman, 1964]. For the band systems treated in this paper, however, the relatively low values of v_{max} involved in many cases, the general agreement between the position of the Condon loci and the occurrence of known bands, and the fact that no molecular constants beyond $\omega_e x_e$ are available in many cases suggest that the data in tables 3 through 10 are probably not too unrealistic.

Another more general point should be made about the realism of Franck-Condon factors and the potentials to which they are appropriate. This concerns the specific use to which $q_{v'v''}$ are put. In many applications they are used as parameters in the smoothing procedure [Fraser, 1954] briefly described below which ensures the cooperative use of *all* of the measured band intensities in the determination of absolute or relative arrays of the transition probability parameters $S_{v'v''}$, $k_{v'v''}$, $f_{v'v''}$, $A_{v'v''}$, $B_{v'v''}$. Such a procedure is superior to calculations of these quantities band by band because of the great difference of relative error from strong bands to weak bands. The smoothing procedure produces a common error range for the whole system. Equations (1) and (2e) lead to the well-known result:

$$I_{v'v''} = KN_{v'} \nu^4 R_e^2 (\bar{r}_{v'v''}) q_{v'v''} \quad (4)$$

where K is a constant of units and geometry and $N_{v'}$

is the population of the level v' . A plot of $(I_{v'v''}/q_{v'v''} v^4)^{1/2}$ versus $\bar{r}_{v'v''}$ (or $\nu_{v'v''}$ or $\lambda_{v'v''}$ to which it is monotonically related [Nicholls and Jarman, 1956; Nicholls, 1965a] for as many v'' progressions ($v' = \text{const.}$) as the measurements of $I_{v'v''}$ allow, delineates the relative variation of $R_e(r)$ with r for each $v' = \text{const.}$ segment. The segments are displaced relative to each other in ordinate because of the $N^{1/2}$ factor. Objective rescaling procedures [Turner and Nicholls, 1954, Hébert and Nicholls, 1961] allow all of the segments to be placed on the same scale and provides the picture of the variation of $R_e(r)$ with r for the whole band system. A least mean squares fit to the resulting points using a simple empirical algebraic form is normally made. The object of this whole procedure is usually less to study $R_e(r)$ for its own sake than to produce a smoothed array of $S_{v'v''}$ (or one of the related transition probability parameters) by the use of equation (1) in which $R_e(\bar{r}_{v'v''})$ is now read band by band from the plot (or calculated from the empirical algebraic form), and the $q_{v'v''}$ —values are those used in producing the plot.

The important quantities in all of this procedure are the end products, the smoothed arrays of $S_{v'v''}^2$ (or of $A_{v'v''}$, $B_{v'v''}$, $f_{v'v''}$, $k_{v'v''}$). They are almost independent (except in the magnitude of relative errors) of the model of potential appropriate to which the $q_{v'v''}$ and $\bar{r}_{v'v''}$ have been calculated because of the *two* compensating ways in which $q_{v'v''}$ has been used in the procedure, (a) once to make the original $(I_{v'v''}/q_{v'v''} v^4)^{1/2}$ versus $\bar{r}_{v'v''}$ plots, and (b) once in the final application of eq (1) to the rescaled plot. $q_{v'v''}$ has been part of a smoothing process. In this type of application where $q_{v'v''}$ is used, compensatingly, twice, the strict realism of the potential to which it is appropriate is thus not as significant as is often claimed. However, in applications where $q_{v'v''}$, or a similar function of vibrational wavefunctions, is used only once, the realism of the potential model becomes very important. Such cases are: (a) The study of $R_e(r)$ per se, (b) the need for a realistic $q_{v'v''}$ array as an approximation to an $S_{v'v''}$ array when no measured $I_{v'v''}$ are available, (c) the study of Condon loci and the position of strong bands [Murty, 1964], (d) the study of derived quantities of vibrational wave functions.

Over 85 arrays of Franck-Condon factors have been calculated using the programme referred to in section 2 for many radiative, excitation and ionization transitions, and about half of them have so far been published. It has been possible to use these arrays to provide the basis for interpolation of $q_{v'v''}$ for transitions which have not yet been treated [Nicholls, 1964c, 1965b]. This is of particular practical importance where the need for $q_{v'v''}$ —values is for order of magnitude estimates such as are required in identification problems. A theoretically justified transition parameter $t = \beta \Delta r_e$ which has a specific value for a band system is used as

interpolation parameter in plots of $q_{v'v''}$ versus t . t varies between 0.02 and 4.7 for the transitions used to make the interpolation plots, and β is the harmonic mean of the coefficients of $(r - r_e)$ of the two Morse potentials.

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² Relative arrays of $S_{v'v''}$ (and related quantities) are often placed on an absolute basis by comparison with an absolute measurement of one of them or its equivalent [Nicholls, 1964a].