ISOTOPE EFFECTS ON VIBRATIONAL TRANSITION PROBABILITIES
IV. ELECTRONIC TRANSITIONS OF ISOTOPIC C_2, CO, CN, H_2, AND CH MOLECULES

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Received May 10, 1965

ABSTRACT

Franck-Condon factors based on Morse potentials are presented for many important electronic transitions of the normal and stable-isotope-labeled molecules C_2, CO, CN, H_2, and CH, for the $v'' = 0$ progression up to $v' = 10$, for the $v' = 0$ progression up to $v'' = 10$, and for the (1,1) band. Appreciable isotope effects on vibrational transition probability are found for all transitions involving large changes in equilibrium internuclear distances, such as the C_2, Phillips and Fox-Herzberg bands, the CO Asundi, Cameron and Hopfield-Birge *a* bands and the H_2, Lyman and Werner bands. Harmonic oscillator Franck-Condon factors for (0,0) transitions of alkali metal hydrides versus deuterides are subject to very large isotope effects.

I. INTRODUCTION

The relative intensity in absorption or emission of vibrational bands in electronic spectra of diatomic molecules is controlled mainly by the Franck-Condon factors, or "overlap integral squared" (Herzberg 1950),

$$q = |\int \psi_{v'} \psi_{v''} d\tau|^2 ,$$

where $\psi_{v'}$ and $\psi_{v''}$ are the vibrational wave functions of vibrational levels v' and v'' of the upper and lower electronic state, respectively, and r is the internuclear distance. It is tentatively assumed in the present work that isotopic substitution will affect mainly the Franck-Condon factor for a given transition, but not the electronic transition moment (Halmann and Laulicht 1965). Spectra of absorption or emission bands of diatomic molecules are important sources of information on the isotopic composition of planetary and stellar atmospheres. It has usually been assumed that isotopic substitution has no effect on band intensities. The purpose of the present work is to find out to what extent this assumption is justified, and in which band systems it will be necessary to apply corrections derived from isotope effects on vibrational transition probability.

II. METHOD

Morse potential functions and Morse wave functions were taken as fairly satisfactory approximations to realistic functions (Nicholls 1961; Ory, Gittleman, and Maddox 1964). Details of the computation program used are being published elsewhere (Halmann and Laulicht 1965). The computer input data were the spectroscopic constants ω_e', ω_e'', $\omega_e' x_i'$, $\omega_e'' x_e''$, r_e' and r_e'' and the reduced masses μ and μ_i of the normal and the isotopic molecules. Molecular constants used are presented in Table 1.

For a number of transitions, in which for a given vibrational level v the value $\omega_e/(\omega_e x_e)$ is smaller than $(2v - 1)$, computation based on Morse functions was not possible. In this case, as well as for a few other band systems, Franck-Condon factors for the (0,0) bands were calculated by a simple harmonic oscillator model, using a program based on the equation reported by Manneback (1951).

III. RESULTS

Franck-Condon factors computed with Morse functions for the normal and isotopically labeled molecules for bands of the $v'' = 0$ and $v' = 0$ progressions, and for the (1,1) band, are presented in Tables 2–26. Franck-Condon factors based on the harmonic oscillator approximation for (0,0) bands are given in Table 27. The last figure in each

entry is a decimal exponent. Wherever available, literature results for Franck-Condon factors of the normal molecule have also been included for comparison.

C_2 Swan Bands (Table 2)

This important band system is a major constituent of the emission spectra of the heads of comets (Stawikowski and Greenstein 1964). Its spectrum has been studied extensively in the laboratory (Jenkins 1948; King 1948; Hagan 1963). Our Franck-Condon factors for the normal molecule, $^{12}C_2$, agree well with those reported by Nicholls, Fraser, and Jarmain (1959), and recently by Ortenberg (1964). The isotope effect on Franck-Condon factors is slight. For the (0,0) band, the ratio $q(^{12}C_2)/q(^{12}C^{13}C)$ amounts only to 1.0063 (see Table 2). Measurements of the intensity of the $^{12}C^{13}C$(1,0) Swan band in a comet (Stawikowski and Greenstein 1964) led to the conclusion that the isotope ratio $^{12}C/^{13}C$ is 70 ± 15. It is thus quite similar to that on the Earth (about 90). This conclusion was based on the assumption that the vibrational transition probability is not affected by isotopic substitution. Within the precision yet available in measurements of emission intensity, this assumption seems justified, as shown by the results in Table 2.

C_2 Fox-Herzberg and Phillips Band Systems (Tables 3 and 4)

In these systems, large differences in equilibrium internuclear separation between the upper and lower states cause a widely spread out vibrational structure. The spectroscopic constants used in the computation of Franck-Condon factors for the Phillips bands (see Table 1) are those recommended by Ballik and Ramsay (1963). Therefore, the values of Franck-Condon factors in the present work differ slightly from those of Nicholls *et al.* (1959) and of Ortenberg (1964), who used Herzberg's (1950) constants. The isotope effect on the (0,0) bands is appreciable. The ratio $q(^{12}C_2)/q(^{12}C^{13}C)$ for the Fox-Herzberg and for the Phillips bands amounts to 1.131 and 1.018, respectively.

C_2 Deslandres-d'Azambuja, Mulliken, Freymark, and Ballik-Ramsay Band Systems (Tables 5–8)

In these band systems of C_2, the equilibrium internuclear distances in the upper and lower states are very similar. Therefore, the most intense transitions are the (0,0) and (1,1) bands, among those treated in the present work. The isotope effect on Franck-Condon factors is very small; for the (0,0) bands, the ratio $q(^{12}C_2)/q(^{12}C^{13}C)$ amounts to 1.0120, 1.0000, 1.0128, and 1.0090, respectively (see Tables 5–8).

CO Fourth Positive, Cameron, Hopfield-Birge a, *and Asundi Band Systems (Tables 9–12)*

The band systems of carbon monoxide, which are easily observed in the laboratory in emission or absorption, seem not to have been detected from extraterrestrial sources. However, photodissociation in the CO_2 atmosphere of Venus may presumably also produce carbon monoxide, which may eventually be detected by spectral observation from outside the Earth's atmosphere. The Franck-Condon factors computed for the fourth positive group, and for the Cameron, Hopfield-Birge *a*, and Asundi bands of $^{12}C^{16}O$ are in good agreement with those reported by Nicholls (1962*a*). The isotope effect is appreciable in all four band systems. For the (0,0) band, the isotope ratio $q(^{12}C^{16}O)q/(^{13}C^{16}O)$ amounts to 1.049, 1.030, 1.220, and 1.078, respectively. Experimental intensity distribution among vibrational bands in the lowest energy transition ($A^1\Pi \leftarrow X^1\Sigma^+$; fourth positive group) of $^{12}C^{16}O$, as determined by electron impact excitation (Silverman and Lassettre 1964; Skerbele and Lassettre 1965), is in agreement with the computed Franck-Condon factors. It should be of interest to use such a technique to study the isotope effects predicted from the present work.

CO^+ Comet-Tail, Baldet-Johnson, and First Negative Band Systems (Tables 13–15)

Emission bands of CO^+ are the major spectral feature of the tails of comets (Herzberg 1950; Swings and Haser 1955) and probably also of the fluorescent emission from the

atmosphere of Venus (Urey and Brewer 1957). Franck-Condon factors for the comet-tail, Baldet-Johnson, and first negative bands of $^{12}C^{16}O^+$, as presented in Tables 13–15, agree well with those reported by Nicholls (1962*a*, *b*). Slight, but appreciable, isotope effects on Franck-Condon factors are found in all three systems. For the (0,0) bands, the ratio $q(^{12}C^{16}O^+)/q(^{13}C^{16}O^+)$ amounts to 1.074, 1.021, and 1.013, respectively. The comet-tail band system, in which a large difference in equilibrium internuclear separation in the upper and lower states causes a very widely spread out vibrational structure, is also subject to the largest isotope effect on Franck-Condon factors. Such an effect should be taken into account, when using spectral intensity data for determination of isotopic abundance in comets and possibly in planetary atmospheres.

CN Red and Violet Band Systems (Tables 16 and 17)

The red and violet CN bands are important spectral constituents of the heads of comets (Stawikowski and Greenstein 1964), and are also the most predominant molecular feature in the visible spectrum of the Sun and of several stellar atmospheres (Herzberg 1950). Bands due to CN have also been identified in the spectrum of lightning (Wallace 1964). The Franck-Condon factors for $^{12}C^{14}N$ for these two band systems, as presented in Tables 16 and 17, are in good agreement with those recently reported by Nicholls (1964). Only the CN red band system, which has a widely spread-out vibrational structure, is subject to an appreciable isotope effect. For the (0,0) band, the ratio $q(^{12}C^{14}N)/q(^{13}C^{14}N)$ amounts to 1.013, while for the violet bands, this ratio is only 1.002. The relative intensity of the red bands of isotopic CN molecules has been used for determination of the ^{12}C:^{13}C ratio in stars (McKellar 1949). For more precise intensity measurements than those which had been possible up to now, the isotope effect on vibrational transition probability will have to be considered.

OH Violet Band System (Table 18)

Bands of OH have been observed in the solar spectrum (Moore and Broida 1957) and by radio observation in the interstellar medium (Weinreb, Barrett, Meeks, and Henry 1963). The oscillator strength of the violet system of OH has been determined by measurements of the radiative lifetime of the transition (Bennett and Dalby 1964). Franck-Condon factors for the violet bands of OH have been reported by Nicholls *et al.* (1959) and agree well with the present results (Table 18). The isotope effect on Franck-Condon factors causes a shift in the weight of vibrational transition probability to higher quantum numbers for OD. The effect of vibration-rotation interaction on transition probability for the violet system of OH and OD has been examined in detail by Learner (1962) and will not be considered here.

H_2 Lyman, Werner, (D–X) and (B′–X) Band Systems (Tables 19–22)

Hydrogen is probably the most abundant molecular constituent in stellar atmospheres (Herzberg 1950). Data on vibrational transition probability for hydrogen and its isotopes will therefore be important for evaluating spectral data which will be obtained by observations from outside the Earth's atmosphere. Franck-Condon factors for several bands of the Lyman and the Werner systems of H_2 have been reported by Patch (1964), who used Morse potential functions, modified by the method of Hulburt and Hirschfelder (1941). In the present work, simple Morse potentials were used, as for the other band systems. A comparison of our results with those of Patch is possible for the (0,2) and (0,3) bands of the Werner system (see Table 20). The Franck-Condon factors calculated with simple Morse potentials agree in order of magnitude with the more realistic factors of Patch. It seems that the simple Morse function Franck-Condon factors should be adequate to indicate the isotope effect on Franck-Condon factors even for an unharmonic molecule such as hydrogen, at least for the lower vibrational levels.

In the Lyman band system, which involves a very large change in equilibrium internuclear separation ($r_e' - r_e'' = 0.55104$ Å), a widely spread out vibrational structure is

found (Table 19). The isotope effect on Franck-Condon factors is extremely large. Thus, for the (0,0) band, the isotope ratio $q(H_2)/q(D_2)$ is 7.47. In passing from H_2 to the heavier isotopic molecules HD, HT, and D_2, the maximum in the vibrational transition probability in the $v'' = 0$ and in the $v' = 0$ progressions is successively shifted to higher levels v' and v'' (see Table 19, in which the maxima are italicized). Thus, in the heavier hydrogen molecules, the Condon parabolae are shifted outward, as compared with that in H_2.

In the Werner band system, which involves a relatively more moderate change in equilibrium internuclear separation ($r_e' - r_e'' = 0.2914$ Å), the isotope effects on Franck-Condon factors are smaller than in the Lyman system but still considerable. For the (0,0) band, the ratio $q(H_2)/q(D_2)$ is 2.42. Similarly, for the (D–X) and the (B'–X) band systems (Tables 21 and 22), which have recently been studied by Monfils (1961) and by Namioka (1964), large isotope effects on Franck-Condon factors are obtained. For the (0,0) band, the ratio $q(H_2)/q(D_2)$ amounts to 2.49 and 3.84, respectively. Such large isotope effects should certainly show up in absorption intensity measurements.

The distribution of intensities of vibrational bands in the electron impact spectrum of HD (Simpson 1964) for the ($B \leftarrow X$) transition seems qualitatively in agreement with the distribution of Franck-Condon factors (Table 19). Absorption coefficients for the ($D \leftarrow X$) bands of H_2 and D_2, as measured by Cook and Metzger (1964) are also in fair agreement with the distribution of Franck-Condon factors for this transition (Table 21).

CH(A–X), (B–X) and (C–X) Band Systems (Tables 23–25)

Emission bands of the ($A^2\Delta$–$X^2\Pi$) system of CH have been observed in the spectrum of the heads of comets, while absorption bands of this system have been detected in the solar atmosphere, and in interstellar space (Herzberg 1950). Bands of CH are the major molecular feature of the spectrum of CH stars, together with C_2 Swan and CN bands (Keenan 1942). Wallerstein and Greenstein (1964) found no positive evidence for the existence of ^{13}CH on their tracings for two CH stars and had to conclude that the carbon is largely ^{12}C.

Vibrational transition probabilities for CH bands have been reported, using a distorted harmonic oscillator approximation (Pillow 1955). Since the change in equilibrium internuclear distance during all three transitions of CH is small, only the (0,0) and (1,1) bands (among those listed in our tables) have a high vibrational transition probability. The isotope effect on Franck-Condon factors is very small. The present results were computed, using the spectroscopic constants listed by Herzberg (1950), which differ only slightly from those of Kiess and Broida (1956) and from those recommended by Garstang (1963).

MgH Green Band System (Table 26)

The green (0,0) and (1,0) bands of magnesium hydride have been identified on the disk of the Sun (Herzberg 1950), and recently together with NaD lines in late K-dwarf spectra (Spinrad 1965). In this band system, the change in equilibrium internuclear distance is rather small. Therefore, only the (0,0) band is prominent. The isotope effect on Franck-Condon factors in changing from MgH to MgD is small (see Table 26), in spite of the large increase in reduced mass.

Harmonic Oscillator Franck-Condon Factors for (0,0) Bands (Table 27)

The A–X transitions of alkali metal hydrides involve very large changes in equilibrium internuclear distance. Thus, the (0,0) bands are of very low intensity and are usually not observed. Nevertheless, it is of interest to present the harmonic oscillator Franck-Condon factors for these bands (see Table 27). The isotope effect on Franck-Condon factors for the alkali metal hybrides is enormous. For rubidium hydride, the ratio $q(RbH)/q(RbD) = 65.2$. Since these molecules are very strongly anharmonic, these Franck-Condon factors are likely not to be very realistic. It should be of considerable interest to find experimental evidence for the relative intensities of the hydride and deuteride bands.

For the various transitions of BH, BN, BO, B_2, and PbO presented in Table 27, the changes in equilibrium internuclear distances are very small. The isotope effects on Franck-Condon factors are very slight.

IV. DISCUSSION

As seen in the tables, large isotope effects on Franck-Condon factors require both a large difference in reduced masses between the normal and the isotopic molecule, as well as a considerable change in equilibrium internuclear distance during the transition. Thus, large isotope effects on vibrational transition probability appear for transitions with a widely spread out vibrational structure. Assuming the electronic transition moment to be independent of isotopic substitution, enormous differences in band intensities can be predicted for a few of the band systems treated in the present work, such as for the alkali metal hydrides, and for the H_2 Lyman and Werner systems. No experimental evidence for these effects seems available.

For the bands systems of C_2, CO, CN, and CH treated in the present work, isotope effects on Franck-Condon factors are rather small, less than a few per cent. Unless very high-precision intensity measurements are available, the isotope effect can be neglected.

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TABLE 1

SPECTROSCOPIC CONSTANTS

State	ω_e(cm^{-1})	$\omega_e x_e$(cm^{-1})	r_e(Å)	Reference
	CH Molecules $\mu(^{12}CH) = 0.93002$; $\mu(^{13}CH) = 0.93563$ $\mu(^{12}CD) = 1.72517$			
$X^2\Pi$	2861.6	64.3	1.1198	Herzberg 1950
$A^2\Delta$	2921.0	90.4	1.1026	
$B^2\Sigma^-$	2542.5	373.8	1.1861	
$C^2\Sigma^+$	2824.1	105.8	1.1132	
	C_2 Molecules $\mu(^{12}C_2) = 6.00194$; $\mu(^{12}C^{13}C) = 6.24276$)			
$x^1\Sigma_g^+$	1854.71	13.340	1.24253	Ballik and Ramsay 1963
$X^1{}^3\Pi_u$	1641.35	11.67	1.31190	
$A^1{}^3\Sigma_g^-$	1470.45	11.19	1.36928	
$b^1\Pi_u$	1608.35	12.078	1.31843	
$A\ ^3\Pi_g$	1788.22	16.440	1.2660	Herzberg 1950
$C^1\Pi_g$	1809.1	15.81	1.2552	Ballik and Ramsay 1963
$B^3\Pi_g$	1106.56	39.26	1.5350	Herzberg 1950
$d^1\Sigma_u^+$	1829.57	13.97	1.2378	
$e^1\Sigma_g^+$	1671.5	40.02	1.2517	
	CO Molecules $\mu(^{12}C^{16}O) = 6.8584$; $\mu(^{13}C^{16}O) = 7.17469$ $\mu(^{12}C^{18}O) = 7.20216$			
$X^1\Sigma^+$	2170.21	13.461	1.12819	Herzberg 1950
$A^1\Pi$	1515.61	17.250	1.2351	
$a^1\ ^3\Sigma^+$	1218.0	9.5	1.3590	
$a^3\Pi_r$	1739.25	14.47	1.2093	
	CO^+ Ions			
$X^2\Sigma^+$	2214.24	15.164	1.11506	Herzberg 1950
$A^2\Pi_i$	1562.06	13.532	1.24368	
$B^2\Sigma^+$	1734.18	27.927	1.16868	
	CN Molecules $\mu(^{12}C^{14}N) = 6.46427$; $\mu(^{12}C^{15}N) = 6.66880$ $\mu(^{13}C^{14}N) = 6.74463$			
$X^2\Sigma^+$	2068.614	13.114	1.17198	Nicholls 1964
$A^2\Pi_i$	1812.33	12.61	1.2296	
$B^2\Sigma^+$	2163.90	20.20	1.1493	
	H_2 Molecules $\mu(H_2) = 0.50407$; $\mu(HD) = 0.67192$ $\mu(HT) = 0.75564$; $\mu(D_2) = 1.00736$			
$X^1\Sigma_g^+$	4395.24	117.995	0.74166	Herzberg 1950
$B^1\Sigma_u^+$	1356.90	19.932	1.29270	
$C^2\Pi_u$	2442.72	67.03	1.0331	
$D^1\Pi_u^-$	2354.0	64.3	1.0506	Namioka 1964
$B^1\ ^1\Sigma_u^+$	2039.52	83.406	1.261	

TABLE 2

FRANCK-CONDON FACTORS FOR THE SWAN ($A^3\Pi_g$–$X^3\Pi_u$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES*

$v'v''$	ORTENBERG (1964)	PRESENT WORK		$v'v''$	ORTENBERG (1964)	PRESENT WORK	
	$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}O$		$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$
0,0	7.35 −1	7.3519−1	7.3056−1	1,1	3.6359−1	3.6357−1	3.5478−1
1,0	2.3963−1	2.3964−1	2.4305−1	0,1	2.1299−1	2.1301−1	2.1604−1
2,0	2.445 −2	2.4459−2	2.5596−2	0,2	4.312 −2	4.3121−2	4.4357−2
3,0	7.1 −4	7.0679−4	7.8912−4	0,3	7.37 −3	7.3698−3	7.6653−3
				0,5	1.6 −4	1.5820−4	1.6764−4
				0,6	2 −5	2.0146−5	2.1672−5

* The minus numbers following the entries represent the powers of 10 by which the corresponding entries should be multiplied.

TABLE 3

FRANCK-CONDON FACTORS FOR THE FOX-HERZBERG ($B^3\Pi_g$–$X^3\Pi_u$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK		$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK	
	$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$		$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$
0,0	2−3	1.4364−3	1.2700−3	1,1	3.6 −2	3.3560−2	3.1006−2
1,0	6−3	4.9163−3	4.4342−3	0,1	1.4 −2	1.2823−2	1.1553−2
2,0	1.1−2	9.7307−3	8.9307−3	0,2	5.3 −2	5.1001−2	4.6925−2
3,0	1.7−2	1.4666−2	1.3668−2	0,3	1.24−1	1.2044−1	1.1341−1
4,0	.....	1.8714−2	1.7684−2	0,4	2.02−1	1.9021−1	1.8368−1
5,0	.....	2.1328−2	2.0411−2	0,5	2.41−1	2.1503−1	2.1334−1
6,0	.....	1.9930−3	2.1107−3	0,6	2.13−1	1.8235−1	1.8613−1
7,0	.....	2.4341−2	2.3728−2	0,7	1.37−1	1.2063−1	1.2676−1
8,0	.....	2.2536−2	2.2249−2	0,8	6.1 −2	6.9119−2	6.3923−2
9,0	.....	1.7744−2	1.7890−2				
10,0	.....	1.4501−2	1.4901−2				

TABLE 4

FRANCK-CONDON FACTORS FOR THE PHILLIPS ($b^1\Pi_u$–$x^1\Sigma_g^+$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	ORTENBERG (1964)	PRESENT WORK		$v'v''$	ORTENBERG (1964)	PRESENT WORK	
	$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$		$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$
0,0	4.1016−1	4.1233−1	4.0515−1	1,1	5.32 −3	5.6524−3	4.0128−3
1,0	3.3151−1	3.3170−1	3.3243−1	0,1	3.9989−1	3.9817−1	3.9902−1
2,0	1.6304−1	1.6206−1	1.6505−1	0,2	1.5563−1	1.5474−1	1.5887−1
3,0	6.365 −2	6.2851−2	6.4861−2	0,3	3.084 −2	3.1093−2	3.2907−2
4,0	2.181 −2	2.1425−2	2.2348−2	0,4	3.28 −3	3.4508−3	3.7982−3
5,0	6.90 −3	6.7585−3	7.1109−3	0,5	1.8 −4	2.0871−4	2.4234−4
6,0	2.08 −3	2.0338−3	2.1533−3	0,6	0	6.4153−6	7.9480−6
7,0	6.1 −4	5.9590−4	6.3456−4				
8,0	1.7 −4	1.8149−4	1.8323−4				

TABLE 5

FRANCK-CONDON FACTORS FOR THE DESLANDRES-D'AZAMBUJA ($c^1\Pi_g$–$b^1\Pi_u$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK		$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK	
	$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$		$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$
0,0	7.39 −1	5.5080−1	5.4422−1	1,1	3.65 −1	9.4307−2	8.7815−2
1,0	2.33 −1	3.5614−1	3.5901−1	0,1	2.14 −1	3.0218−1	3.0463−1
2,0	2.7 −2	8.4099−2	8.7091−2	0,2	4.0 −2	1.0620−1	1.0872−1
3,0	1 −3	8.616 −3	9.2813−3	0,3	6 −3	3.0538−2	3.1648−2
4,0	.....	3.4253−4	3.9474−4	0,4	1 −3	7.8481−3	8.2139−3
5,0	.....	2.6829−6	3.7305−6	0,5	.....	1.8806−3	1.9842−3
				0,6	.....	4.3050−4	4.5650−4

TABLE 6

FRANCK-CONDON FACTORS FOR THE ($d^1\Sigma_u^+$–$x^1\Sigma_g^+$) MULLIKEN BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK		$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK	
	$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$		$^{12}C_2$	$^{12}C_2$	$^{12}C^{13}C$
0,0	9.97 −1	9.9659−1	9.9652−1	1,1	9.91 −1	9.9055−1	9.9033−1
1,0	3 −3	3.3148−3	3.3883−3	0,1	3 −3	3.2067−3	3.2777−3
2,0	.....	9.7199−5	9.6246−5	0,2	.....	1.9741−4	1.9892−4
3,0	.....	3.6891−7	3.3513−7	0,3	.....	7.8375−6	7.8381−6
4,0	.....	2.5232−9	2.9857−9	0,4	.....	4.0421−7	4.0034−7

TABLE 7

FRANCK-CONDON FACTORS FOR THE FREYMARK (1951) ($e^1\Sigma_g^+$–$b^1\Pi_u$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	$^{12}C_2$	$^{12}C^{13}C$	$v'v''$	$^{12}C_2$	$^{12}C^{13}C$
0,0	5.7408−1	5.6682−1	1,1	1.5930−1	1.4956−1
1,0	3.7961−1	3.8379−1	0,1	2.7274−1	2.7559−1
2,0	4.5978−2	4.9049−2	0,2	1.0497−1	1.0747−1
3,0	.....	.....	0,3	3.4386−2	3.5614−2
4,0	3.1715−4	3.3198−4	0,4	1.0177−2	1.0646−2
5,0	6.5124−6	4.3561−6	0,5	2.7604−3	2.9163−3
6,0	2.0697−6	2.5756−6	0,6	6.8987−4	7.3559−4

TABLE 8

FRANCK-CONDON FACTORS FOR THE BALLIK-RAMSAY ($A'\ ^3\Sigma_g^- - X'\ ^3\Pi_u$) BAND SYSTEM OF ISOTOPIC C_2 MOLECULES

$v'v''$	$^{12}C_2$	$^{12}C^{13}C$	$v'v''$	$^{12}C_2$	$^{12}C^{13}C$
0,0.....	6.3243−1	6.2673−1	1,1.....	1.8543−1	1.7768−1
1,0.....	2.7092−1	2.7381−1	0,1.....	3.0664−1	3.0990−1
2,0.....	7.4853−2	7.6793−2	0,2.....	5.5915−2	5.7976−2
3,0.....	1.7242−2	1.7890−2	0,3.....	4.8126−3	5.1645−3
4,0.....	3.6368−3	3.8054−3	0,4.....	2.0071−4	2.2604−4
5,0.....	7.3518−4	7.7392−4	0,5.....	3.7017−6	4.4788−6
6,0.....	1.4627−4	1.5468−4	0,6.....	1.9711−8	2.9682−8

TABLE 9

FRANCK-CONDON FACTORS FOR THE FOURTH POSITIVE ($A^1\Pi - X^1\Sigma^+$) BAND SYSTEM OF ISOTOPIC CO MOLECULES

$v'v''$	NICHOLLS (1962a)	PRESENT WORK			$v'v''$	NICHOLLS (1962a)	PRESENT WORK		
	$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$		$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$
0,0..	1.1319−1	1.1313−1	1.0783−1	1.0739−1	1,1...	1.5487−1	1.5492−1	1.5958−1	1.5997−1
1,0..	2.1614−1	2.1607−1	2.1052−1	2.1005−1	0,1...	2.6087−1	2.6081−1	2.5405−1	2.5347−1
2,0..	2.2997−1	2.2995−1	2.2848−1	2.2836−1	0,2...	2.8477−1	2.8477−1	2.8384−1	2.8375−1
3,0..	1.8128−1	1.8130−1	1.8332−1	1.8348−1	0,3...	1.9629−1	1.9633−1	2.0049−1	2.0083−1
4,0..	1.1879−1	1.1882−1	1.2200−1	1.2227−1	0,4...	9.6040−2	9.6077−2	1.0065−1	1.0104−1
5,0..	6.8846−2	6.8882−2	7.1669−2	7.1908−2	0,5...	3.5535−2	3.5555−2	3.8262−2	3.8500−2
6,0..	3.6675−2	3.6702−2	3.8624−2	3.8791−2	0,6...	1.0340−2	1.0352−2	1.1459−2	1.1552−2
7,0..	1.8429−2	1.8565−2	1.9717−2	1.9821−2	0,7...	2.4282−3	2.4187−3	2.7874−3	2.8137−3
8,0..	8.8974−3	8.9615−3	9.6006−3	9.6461−3	0,8...	4.6859−4	4.6591−4	5.3113−4	6.0376−4
9,0..	4.1842−3	4.1804−3	4.4871−3	4.5280−3	9,0...	7.5264−5	.....	.....	.....
10,0..	1.9367−3	1.9388−3	2.0110−3	2.0685−3					

TABLE 10

FRANCK-CONDON FACTORS FOR THE CAMERON ($a^3\Pi - X^1\Sigma^+$) BAND SYSTEM OF ISOTOPIC CO MOLECULES

$v'v''$	NICHOLLS (1962a)	PRESENT WORK			$v'v''$	NICHOLLS (1962a)	PRESENT WORK		
	$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$		$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$
0,0...	2.6630−1	2.6620−1	2.5842−1	2.3152−1	1,1...	2.8773−2	2.8829−2	3.3191−2	3.3573−2
1,0...	3.1901−1	3.1897−1	3.1663−1	3.1643−1	0,1...	3.7840−1	3.7837−1	3.7555−1	3.7530−1
2,0...	2.1889−1	2.1892−1	2.2156−1	2.2178−1	0,2...	2.3951−1	2.3956−1	2.4374−1	2.4409−1
3,0...	1.1396−1	1.1401−1	1.1732−1	1.1860−1	0,3...	8.9476−2	8.9519−2	9.3647−2	9.4001−2
4,0...	5.0350−2	5.0385−2	5.2594−2	5.2785−2	0,4...	2.2038−2	2.2055−2	2.3799−2	2.3952−2
5,0...	2.0031−2	2.0050−2	2.1182−2	2.1281−2	0,5...	3.7861−3	3.8904−3	4.2349−3	4.2743−3
6,0...	7.4386−3	7.4481−3	7.9465−3	7.9912−3	0,6...	4.6808−4	4.6996−4	5.4578−4	5.5121−4
7,0...	2.6402−3	2.6518−3	2.8557−3	2.8695−3					
8,0...	.....	9.0778−4	9.7816−4	9.9953−4					
9,0...	.....	3.0604−4	3.4225−4	3.1591−4					

TABLE 11

FRANCK-CONDON FACTORS FOR THE HOPFIELD-BIRGE a ($a'\ ^3\Sigma^+ - X^1\Sigma^+$) BAND SYSTEM OF ISOTOPIC CO MOLECULES

$v'v''$	NICHOLLS (1962a)	PRESENT WORK			$v'v''$	NICHOLLS (1962a)	PRESENT WORK		
	$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$		$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$	$^{12}C^{18}O$
0,0	1.5607−4	1.5482−4	1.2693−4	1.2479−4	1,1	8.8725−3	8.8199−3	7.6049−3	7.5083−3
1,0	1.0767−3	1.0688−3	8.9624−4	8.8278−4	0,1	1.6277−3	1.6165−3	1.3552−3	1.3348−3
2,0	3.9031−3	3.8774−3	3.3220−3	3.2780−3	0,2	8.1812−3	8.1342−3	6.9791−3	6.8877−3
3,0	9.9038−3	9.8454−3	8.6091−3	8.5100−3	0,3	2.6351−2	2.6228−2	2.3054−2	2.2798−2
4,0	1.9768−2	1.9665−2	1.7533−2	1.7359−2	0,4	6.1009−2	6.0791−2	5.4801−2	5.4310−2
5,0	3.3075−2	3.2925−2	2.9901−2	2.9652−2	0,5	1.0798−1	1.0771−1	9.9705−2	9.9033−2
6,0	4.8277−2	4.8091−2	4.4445−2	4.4141−2	0,6	1.5170−1	1.5148−1	1.4420−1	1.4356−1
7,0	6.3177−2	6.3154−2	5.9334−2	5.9011−2	0,7	1.7343−1	1.7365−1	1.7024−1	1.6991−1
8,0	7.5605−2	7.5417−2	7.1986−2	7.1691−2	0,8	1.6416−1	1.6416−1	1.6608−1	1.6627−1

TABLE 12

FRANCK-CONDON FACTORS FOR THE ASUNDI ($a'^3\Sigma^+ - a^3\Pi_r$) BAND SYSTEM OF ISOTOPIC CO MOLECULES

$v'v''$	JARMAIN *et al.* (1955)	PRESENT WORK		$v'v''$	JARMAIN *et al.* (1955)	PRESENT WORK	
	$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$		$^{12}C^{16}O$	$^{12}C^{16}O$	$^{13}C^{16}O$
0,0	3.7 −2	3.7221−2	3.4527−2	1,1	1.95−1	1.9335−1	1.9139−1
1,0	1.03−1	1.0510−1	9.9738−2	0,1	1.43−1	1.4215−1	1.3487−1
2,0	1.62−1	1.6199−1	1.5695−1	0,2	2.43−1	2.4786−1	2.4105−1
3,0	1.81−1	1.8084−1	1.7857−1	0,3	.....	2.6001−1	2.5990−1
4,0	1.65−1	1.6383−1	1.6462−1	0,4	.....	1.8214−1	1.8775−1
5,0	1.29−1	1.2800−1	1.3069−1	0,5	.....	8.9475−2	9.5519−2
6,0	9.1 −2	8.9534−2	9.2772−2	0,6	.....	3.1510−2	3.5023−2
7,0	5.9 −2	5.7667−2	6.0546−2	0,7	.....	8.0177−3	9.3387−3
8,0	.....	3.4647−2	3.6753−2	0,8	.....	1.4532−3	1.7728−3
9,0	.....	1.9619−2	2.1276−2				
10,0	.....	1.0811−2	1.211 −2				

TABLE 13

FRANCK-CONDON FACTORS FOR THE ($A^2\Pi_i - X^2\Sigma^+$) COMET-TAIL BAND SYSTEM OF ISOTOPIC CO^+ IONS

$v'v''$	NICHOLLS (1962b)	PRESENT WORK			$v'v''$	NICHOLLS (1962b)	PRESENT WORK		
	$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$		$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$
0,0	4.2745−2	4.2697−2	3.9762−2	3.9520−2	1,1	1.9325−1	1.9324−1	1.9201−1	1.9189−1
1,0	1.1506−1	1.1497−1	1.0950−1	1.0904−1	0,1	1.5201−1	1.5190−1	1.4465−1	1.4404−1
2,0	1.6979−1	1.6970−1	1.6498−1	1.6457−1	0,2	2.4987−1	2.4979−1	2.4368−1	2.4315−1
3,0	1.8244−1	1.8240−1	1.8065−1	1.8049−1	0,3	2.5157−1	2.5159−1	2.5196−1	2.5197−1
4,0	1.6004−1	1.6005−1	1.6122−1	1.6131−1	0,4	1.7335−1	1.7342−1	1.7873−1	1.7917−1
5,0	1.2187−1	1.2192−1	1.2470−1	1.2493−1	0,5	8.6541−2	8.6609−2	9.2114−2	9.2586−2
6,0	8.3692−2	8.3748−2	8.6847−2	8.7112−2	0,6	3.2330−2	3.2369−2	3.5643−2	3.5931−2
7,0	5.3165−2	5.3405−2	5.6062−2	5.6290−2	0,7	9.2074−3	9.2408−3	1.0575−2	1.0695−2
8,0	3.1817−2	3.1837−2	3.3812−2	3.3940−2	0,8	2.0181−3	2.0809−3	2.5225−3	2.3584−3

TABLE 14

FRANCK-CONDON FACTORS FOR THE BALDET-JOHNSON ($B^2\Sigma^+$–$A^2\Pi_i$) BAND SYSTEM OF ISOTOPIC CO^+ IONS

$v'v''$	NICHOLLS (1962b)	PRESENT WORK			$v'v''$	NICHOLLS (1962b)	PRESENT WORK		
	$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$		$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$
0,0	4.1496−1	4.1514−1	4.0638−1	4.0483−1	1,1	1.1762−2	1.1826−2	8.7676−3	8.2737−3
1,0	4.3277−1	4.3271−1	4.3405−1	4.3426−1	0,1	3.1478−1	3.1470−1	3.1562−1	3.1577−1
2,0	1.3906−1	1.3895−1	1.4474−1	1.4577−1	0,2	1.6116−1	1.6110−1	1.6443−1	1.6502−1
3,0	1.3129−2	1.3106−2	1.4695−2	1.4990−2	0,3	6.8711−2	6.8658−2	7.1062−2	7.1494−2
4,0	7.0428−5	6.9978−5	1.1770−4	1.2784−4	0,4	2.6328−2	2.6299−2	2.7534−2	2.7758−2
5,0	2.6197−5	2.6170−5	2.5570−5	2.5387−5	0,5	9.4074−3	9.3933−3	9.9298−3	1.0028−2
6,0	1.7089−7	1.6946−7	3.7430−7	4.1905−7	0,6	3.1995−3	3.1934−3	3.4034−3	3.4429−3

TABLE 15

FRANCK-CONDON FACTORS FOR THE FIRST NEGATIVE ($B^2\Sigma^+$–$X^2\Sigma^+$) BAND SYSTEM OF ISOTOPIC CO^+ IONS

$v'v''$	NICHOLLS (1962b)	PRESENT WORK			$v'v''$	NICHOLLS (1962b)	PRESENT WORK		
	$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$		$^{12}C^{16}O^+$	$^{12}C^{16}O^+$	$^{13}C^{16}O^+$	$^{12}C^{18}O^+$
0,0	5.3146−1	5.3120−1	5.2431−1	5.2373−1	1,1	5.6508−2	5.6317−2	5.1380−2	5.0970−2
1,0	3.1251−1	3.1257−1	3.1495−1	3.1515−1	0,1	3.3935−1	3.3946−1	3.4197−1	3.4218−1
2,0	1.1150−1	1.1161−1	1.1434−1	1.1458−1	0,2	1.0391−1	1.0401−1	1.0703−1	1.0729−1
3,0	3.2473−2	3.2528−2	3.3740−2	3.3845−2	0,3	2.1425−2	2.1455−2	2.2525−2	2.2618−2
4,0	8.7613−3	8.7826−3	9.1831−3	9.2180−3	0,4	3.3829−3	3.3889−3	3.6273−3	3.6481−3
5,0	2.3512−3	2.3585−3	2.4751−3	2.4853−3	0,5	4.3283−4	4.3371−4	4.7353−4	4.7692−4
6,0	6.5484−4	6.5728−4	6.8944−4	6.9228−4	0,6	4.6493−5	4.6701−5	5.1950−5	5.2445−5

TABLE 16

FRANCK-CONDON FACTORS FOR THE RED BAND SYSTEM ($A^2\Pi_i$–$X^2\Sigma^+$) OF ISOTOPIC CN MOLECULES

$v'v''$	NICHOLLS (1964)	PRESENT WORK			$v'v''$	NICHOLLS (1964)	PRESENT WORK		
	$^{12}C^{14}N$	$^{12}C^{14}N$	$^{12}C^{15}N$	$^{13}C^{14}N$		$^{12}C^{14}N$	$^{12}C^{14}N$	$^{12}C^{15}N$	$^{13}C^{14}N$
0,0	5.3757−1	5.3755−1	5.3238−1	5.3050−1	1,1	7.6745−2	7.6729−2	7.2159−2	7.0528−2
1,0	3.1160−1	3.1161−1	3.1344−1	3.1410−1	0,1	3.5349−1	3.5349−1	3.5555−1	3.5629−1
2,0	1.0995−1	1.0996−1	1.1201−1	1.1276−1	0,2	9.4547−2	9.4550−2	9.6914−2	9.7781−2
3,0	3.0917−2	3.0922−2	3.1821−2	3.2154−2	0,3	1.3294−2	1.3295−2	1.3949−2	1.4193−2
4,0	7.6765−3	7.6779−3	7.9662−3	8.0735−3	0,4	1.0612−3	1.0612−3	1.1467−3	1.1792−3
5,0	1.7727−3	1.7731−3	1.8517−3	1.8810−3	0,5	4.8473−5	4.8476−5	5.4429−5	5.6707−5
6,0	3.9235−4	3.9309−4	4.1234−4	4.1907−4					
7,0	8.4825−5	.....	.....	.....					
8,0	1.8149−5	1.8146−5	1.9161−5	1.9546−5					

TABLE 17

FRANCK-CONDON FACTORS FOR THE VIOLET BAND SYSTEM ($B^2\Sigma^+$–$X^2\Sigma^+$) OF ISOTOPIC CN MOLECULES

$v'v''$	NICHOLLS (1964)	PRESENT WORK			$v'v''$	NICHOLLS (1964)	PRESENT WORK		
	$^{12}C^{14}N$	$^{12}C^{14}N$	$^{12}C^{15}N$	$^{13}C^{14}N$		$^{12}C^{14}N$	$^{12}C^{14}N$	$^{12}C^{15}N$	$^{13}C^{14}N$
0,0	9.0861−1	9.0860−1	9.0712−1	9.0658−1	1,1	7.5682−1	7.5680−1	7.5286−1	7.5142−1
1,0	8.9808−2	8.9809−2	9.1203−2	9.1713−2	0,1	8.3968−2	8.3975−2	8.5275−2	8.5752−2
2,0	1.5782−3	1.5781−3	1.6685−3	1.7023−3	0,2	6.9510−3	6.9519−3	7.1183−3	7.1797−3
3,0	7.8971−6	7.8988−6	6.8697−6	6.5054−6	0,3	4.4870−4	4.4878−4	4.6409−4	4.6978−4
4,0	8.6112−7	8.6074−7	9.1690−7	9.3688−7	0,4	1.9898−5	1.9905−5	2.0953−5	2.1348−5
5,0	1.1289−8	.....	.....	.....	0,5	2.7721−7	2.7735−7	3.1544−7	3.3372−7
6,0	7.2137−10	.....	.....	.....	0,6	2.6248−8	2.4423−8	1.5841−8	5.2589−9
7,0	1.0162−10	.....	.....	.....					
8,0	2.2048−12	2.1579−12	1.5892−12	1.4080−12					

TABLE 18

FRANCK-CONDON FACTORS FOR THE VIOLET ($A^2\Sigma$–$X^2\Pi$) BAND SYSTEM OF ISOTOPIC OH MOLECULES

$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK		$v'v''$	NICHOLLS *et al.* (1959)	PRESENT WORK	
	^{16}OH	^{16}OH	^{18}OD		^{16}OH	^{16}OH	^{16}OD
0,0	9.07−1	9.0702−1	8.7383−1	1,1	7.17−1	7.1383 −1	6.3100−1
1,0	8.6 −2	8.5974−2	1.1426−1	0,1	8.9 −2	8.9348 −2	1.1918−1
2,0	6 −3	6.4976−3	1.0848−2	0,2	3 −3	3.5821 −3	6.7880−3
3,0	.....	4.7473−4	9.6065−4	0,3	.....	5.3800 −5	1.9994−4
4,0	.....	3.4849−5	8.7746−5				

TABLE 19

FRANCK-CONDON FACTORS FOR THE LYMAN ($B^1\Sigma_u^+$–$X^1\Sigma_g^+$) BAND SYSTEM OF ISOTOPIC HYDROGEN MOLECULES

$v'v''$	H_2	HD	HT	D_2	$v'v''$	H_2	HD	HT	D_2
0,0	6.8149−3	3.1972−3	2.2344−3	9.1240−4	1,1	9.7587−2	6.5381−2	5.2244−2	2.9667−2
1,0	3.0537−2	1.6261−2	1.2308−2	5.6194−3	0,1	3.4749−2	1.9184−2	1.3768−2	6.6384−3
2,0	7.1712−2	4.3262−2	3.5203−2	1.7986−2	0,2	9.6578−2	6.1701−2	4.5834−2	2.5633−2
3,0	1.1731−1	8.0080−2	6.9543−2	3.9822−2	0,3	1.7869−2	1.3246−1	1.0340−1	6.6831−2
4,0	1.4987−1	1.1575−1	1.0651−1	6.8508−2	0,4	*2.3454−1*	2.0407−1	1.7102−1	1.2812−1
5,0	*1.5893−1*	1.3899−1	1.3455−1	1.7517−2	0,5	2.2063−1	*2.3025−1*	*2.1350−1*	1.8706−1
6,0	1.4511−1	*1.4404−1*	*1.4564−1*	1.1943−1	0,6	1.4551−1	1.8877−1	2.0204−1	*2.1028−1*
7,0	1.1809−1	1.3338−1	1.3949−1	1.3008−1	0,7	6.6905−2	1.1331−1	1.4723−1	1.8658−1
8,0	8.4929−2	1.1012−1	1.1847−1	1.2663−1	0,8	1.7443−2	4.3078−2	7.5464−2	1.2013−1
9,0	5.4360−2	8.1987−2	9.0204−2	1.1167−1					
10,0	3.1676−2	5.6494−2	6.2836−2	9.1280−2					

TABLE 20

FRANCK-CONDON FACTORS FOR THE WERNER ($C^1{}_u$–$X^1\Sigma_g{}^+$) BAND SYSTEM OF ISOTOPIC HYDROGEN MOLECULES

$v'v''$	PRESENT WORK				$v'v''$	PATCH (1964)	PRESENT WORK			
	H_2	HD	HT	D_2		H_2	H_2	HD	HT	D_2
0,0	1.2617−1	9.0422−2	7.9739−2	5.2189−2	1,1	.....	1.3745−1	1.6820−1	1.7843−1	1.9000−1
1,0	2.0928−1	1.6363−1	1.6254−1	1.2007−1	0,1	.....	3.1047−1	2.6567−1	2.3907−1	1.8754−1
2,0	2.0839−1	1.7947−1	1.9232−1	1.5976−1	0,2	2.700−1	3.2485−1	3.2868−1	3.1575−1	2.9607−1
3,0	1.6351−1	1.5659−1	1.7428−1	1.6234−1	0,3	1.236−1	1.7832−1	2.1696−1	2.3313−1	2.6386−1
4,0	1.1235−1	1.2070−1	1.3490−1	1.4059−1	0,4	.....	5.2305−2	8.0429−2	1.0220−1	1.4289−1
5,0	7.1395−2	8.6704−2	9.4443−2	1.0993−1	0,5	.....	7.4924−3	1.6212−2	2.6246−2	4.7318−2
6,0	4.3346−2	5.9887−2	6.1918−2	8.0374−2	0,6	.....	3.9161−4	1.5697−3	3.6411−3	9.1711−3
7,0	2.7043−2	4.3578−2	4.0120−2	5.8017−2						
8,0	1.5861−2	2.9272−2	2.4540−2	3.9469−2						
9,0	8.8352−3	1.8274−2	1.4338−2	2.5602−2						
10,0	5.2200−3	1.2272−2	8.5886−3	1.7003−2						

TABLE 21

FRANCK-CONDON FACTORS FOR THE ($D^1\Pi_u$–$X^1\Sigma_g{}^+$) TRANSITION OF ISOTOPIC HYDROGEN MOLECULES

$v'v''$	H_2	HD	D_2	$v'v''$	H_2	HD	D_2
0,0	1.0245−1	7.3102−2	4.1175−2	1,1	1.5901−1	1.8238−1	1.9009−1
1,0	1.8578−1	1.5238−1	1.0555−1	0,1	2.7830−1	2.3114−1	1.5829−1
2,0	1.9993−1	1.8476−1	1.5291−1	0,2	3.2710−1	3.1941−1	2.7399−1
3,0	1.6797−1	1.7183−1	1.6564−1	0,3	2.0632−1	2.4227−1	2.7365−1
4,0	1.2259−1	1.3665−1	1.4998−1	0,4	7.1902−2	1.0558−1	1.6968−1
5,0	8.2189−2	9.8389−2	1.2044−1	0,5	1.2940−2	2.5434−2	6.5827−2
6,0	5.2333−2	6.6389−2	8.8928−2				
7,0	3.4044−2	4.4525−2	6.3189−2				
8,0	2.0738−2	2.8068−2	4.2117−2				
9,0	1.1955−2	1.6827−2	2.6668−2				
10,0	7.2793−3	1.0400−2	1.6905−2				

TABLE 22

FRANCK-CONDON FACTORS FOR THE ($B'\,{}^1\Sigma_u{}^+$–$X^1\Sigma_g{}^+$) TRANSITION OF ISOTOPIC HYDROGEN MOLECULES

$v'v''$	H_2	HD	D_2	$v'v''$	H_2	HD	D_2
0,0	3.3808−3	2.0465−2	8.8183−3	1,1	1.7076−1	1.5113−1	1.0840−1
1,0	7.7394−2	5.4256−2	2.8721−2	0,1	1.4301−1	9.9148−2	5.1814−2
2,0	1.0537−1	8.3695−2	5.2999−2	0,2	2.6716−1	2.1618−1	1.3999−1
3,0	1.1227−1	9.9184−1	7.3402−2	0,3	2.8288−1	2.7508−1	2.2774−1
4,0	1.0404−1	1.0068−1	8.5336−2	0,4	1.8244−1	2.2255−1	2.4602−1
5,0	8.8387−2	9.2602−2	8.8347−2	0,5	7.2000−2	1.1735−1	1.8393−1
6,0	7.0802−2	7.9707−2	8.4402−2	0,6	1.6605−2	3.9867−2	9.6370−2
7,0	6.3272−2	7.2546−2	8.0798−2	0,7	2.1042−3	8.6216−3	3.5864−2
8,0	4.6242−2	5.7441−2	6.9891−2				
9,0	2.7121−2	3.9590−2	5.5179−2				
10,0	1.6346−2	2.9004−2	4.5034−2				

TABLE 23

FRANCK-CONDON FACTORS FOR THE ($A^2\Delta$–$X^2\Pi$) BAND SYSTEM OF ISOTOPIC CH MOLECULES

$v'v''$	^{12}CH	^{13}CH	^{12}CD	$v'v''$	^{12}CH	^{13}CH	^{12}CD
0,0.....	9.9231−1	9.9228−1	9.9150−1	1,1.....	9.8428−1	9.8419−1	9.8103−1
1,0.....	7.4534−3	7.4883−3	8.3735−3	0,1.....	7.1750−3	7.2082−3	8.0970−3
2,0.....	2.2737−4	2.2657−4	1.1432−4	0,2.....	5.0409−4	5.0502−4	3.9667−4

TABLE 24

FRANCK-CONDON FACTORS FOR THE ($B^2\Sigma^-$–$X^2\Pi$) BAND SYSTEM OF ISOTOPIC CH MOLECULES

$v'v''$	^{12}CH	^{13}CH	^{12}CD	$v'v''$	^{12}CH	^{13}CH	^{12}CD
0,0.....	7.0424−1	7.0401−1	7.6576−1	1,1.....	1.2394−1	1.2407−1	2.2672−1
1,0.....	1.5576−1	1.5603−1	1.5542−1	0,1.....	.....	.....	.....
2,0.....	3.7924−2	3.8139−2	3.6974−2	0,2.....	2.7839−2	2.7885−2	2.1987−2
3,0.....	7.7021−3	7.4236−3	1.0179−2				

TABLE 25

FRANCK-CONDON FACTORS FOR THE ($C^2\Sigma^+$–$X^2\Pi$) BAND SYSTEM OF ISOTOPIC CH MOLECULES

$v'v''$	^{12}CH	^{13}CH	^{12}CD	$v'v''$	^{12}CH	^{13}CH	^{12}CD
0,0.....	9.9973−1	9.9973−1	9.9984−1	0,1.....	1.5715−5	1.6699−5	1.6512−7
				0,2.....	2.3537−4	2.3529−4	1.4238−4
				0,3.....	6.2895−6	6.2819−6	1.1323−5
				0,4.....	5.9054−6	5.8833−6	4.8342−6

TABLE 26

FRANCK-CONDON FACTORS FOR THE GREEN ($A^2\Pi_i$–$X^2\Sigma^+$) BAND SYSTEM OF ISOTOPIC MAGNESIUM HYDRIDE MOLECULES

$v'v''$	^{24}MgH	^{24}MgD	$v'v''$	^{24}MgH	^{24}MgD
0,0.....	9.4831−1	9.2459−1	1,1.....	8.6068−1	7.8694−1
1,0.....	5.1589−2	7.4510−2	0,1.....	4.7943−2	6.9439−2
2,0.....	6.7427−5	8.9970−4	0,2.....	3.4896−3	5.4652−3

TABLE 27

FRANCK-CONDON FACTORS FOR (0,0) TRANSITIONS OF VARIOUS ISOTOPIC MOLECULES*

Molecule	Transition	$q(0,0)$	q (light)/q (heavy)
^{7}LiH ^{7}LiD	$A^1\Sigma^+-X^1\Sigma^+$	3.6346−3 6.2419−4	5.82
^{23}NaH ^{23}NaD	$A^1\Sigma^+-X^1\Sigma^+$	3.8442−6 1.3966−6	2.75
^{39}KH ^{39}KD	$A^1\Sigma^+-X^1\Sigma^+$	1.5237−5 3.8285−7	39.8
^{85}RbH ^{85}RbD	$A^1\Sigma^+-X^1\Sigma^+$	2.7167 5 4.1692 7	65.2
^{133}CsH ^{133}CsD	$A^1\Sigma^+-X^1\Sigma^+$	7.0581−5 1.5764−6	44.8
$^{6}Li^{7}Li$ $^{7}Li_2$	$A^1\Sigma_u^+-X^1\Sigma_g^+$	6.0009−2 5.3536−2	1.120
$^{35}Cl_2$ $^{35}Cl^{37}Cl$	$A^3\Pi-X^1\Sigma_g^+$	1.4607−9 1.2671−9	1.152

Molecule	Transition	$q(0,0)$ Present Work	$q(0,0)$ Nicholls *et al.* (1959)	q (light)/q (heavy)
^{10}BH ^{11}BH ^{11}BD	$B^1\Sigma^+-A^1\Pi$	9.9617−1 9.9615−1 9.9480−1	..... 9.9 −1	..... 1.000 1.001
$^{10}B^{14}N$ $^{11}B^{14}N$	$A^3\Pi-X^3\Pi$	7.7403−1 7.6856−1	..... 7.59 −1	..... 1.007
$^{12}B^{16}O$ $^{11}B^{16}O$ $^{11}B^{18}O$	$A^2\Pi_i-X^2\Sigma^+$	4.4693−2 4.0800−2 3.7863−2	..... 3.7 −2	..... 1.095 1.180
$^{10}B^{16}O$ $^{11}B^{16}O$ $^{11}B^{18}O$	$B^2\Sigma^+-A^2\Pi_i$	8.1502−1 8.1012−1 8.0612−1	..... 7.78 −1	..... 1.006 1.011
$^{10}B^{16}O$ $^{11}B^{16}O$ $^{11}B^{18}O$	$B^2\Sigma^+-X^2\Sigma^+$	1.9572−1 1.8663−1 1.7949−1	..... 2.04 −1	..... 1.048 1.090
$^{10}B_2$ $^{11}B_2$	$A^3\Sigma_u^--X^3\Sigma_g^-$	9.0336−1 8.9899−1	..... 9.2 −1	..... 1.004
$^{206}Pb^{16}O$ $^{208}Pb^{16}O$ $^{208}Pb^{18}O$ $^{206}Pb^{18}O$	$A-X^1\Sigma^+$	2.1993−2 2.1982−2 1.7771−2 1.7799−2	2.3 −2	..... 1.0005 1.2376 1.2356
$^{206}Pb^{16}O$ $^{208}Pb^{16}O$ $^{208}Pb^{18}O$ $^{206}Pb^{18}O$	$D-X^1\Sigma^+$	1.1654−1 1.1651−1 1.0334−1 1.0343−1	....	..... 1.0003 1.1278 1.1268

* Molecular constants were taken from Herzberg's compilation (1950).