

The Spectrum of Potassium Hydride

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The ${}^1\Sigma \rightarrow {}^1\Sigma$ molecular spectrum extending from 4100Å to 6600Å has been photographed with prism spectrographs with a d.c. potassium arc in hydrogen as source. In absorption spectrographs, also attempted, the bands were masked by alkali bands except in a short region, 4600Å to 4800Å. The spectrum is of the many-lined type. Analysis disclosed 29 bands falling into five v' progressions. Each band consists of P and R branches only. The rotational and vibrational constants (Table III), which fall into line with the corresponding values for LiH and NaH, are surprisingly different in the two states. B_v' and ω_v' show an anomaly, rising with increasing v' for low values of v' , then decreasing. Extrapolation of the vibrational levels indicates that the products of dissociation in the two states differ by the energy of the resonance lines of K(1.60 volts). Heats of dissociation of 1.25 and 2.06 volts are obtained for the excited and ground states, respectively. From potential energy curves a Franck-Condon diagram of intensity is drawn and is in good agreement with observed intensities.

THE molecular spectra of two of the diatomic hydrides have already been analyzed and reported; Nakamura¹ examined the spectrum of LiH as obtained in absorption while Hori² has made an extensive study of NaH in both absorption and emission. Most of the LiH spectrum falls between 3000Å and 4500Å, that of NaH between 3500Å and 5000Å. The two spectra, which are of the many-lined type, are much alike and have been assigned in each case to a ${}^1\Sigma \rightarrow {}^1\Sigma$ transition. Extrapolation of the vibrational levels of the two states of an alkali hydride indicated as the products of dissociation a normal hydrogen atom and a normal alkali atom from the lower state and a normal hydrogen and an excited 2P alkali atom from the upper state. In this paper the analysis of the corresponding ${}^1\Sigma \rightarrow {}^1\Sigma$ system of KH, obtained in emission and extending from 4100Å to 6600Å, is discussed.

A point of interest in the alkali hydrides is the anomalous behavior of ω_v' , the vibrational interval in the upper state. Instead of decreasing steadily with increasing v' in the usual way, it rises, attains a maximum at about $v'=9$, and then falls. This peculiar behavior is found in KH, as well as in LiH and NaH.

EXPERIMENTAL PROCEDURE

The source of the KH spectrum was a d.c. potassium arc operating in hydrogen. The arc was contained in a brass chamber, cooled by water circulating in a lead tube coiled about it. The electrodes, also water-cooled, were fixed into the removable top and bottom plates. The lower electrode was a hollow iron cylinder of about 1 cm internal diameter, with an iron cap having a 4 mm hole in its center. In the cylinder was a piston with a threaded shaft

¹ G. Nakamura, *Zeits. f. Physik* **59**, 218 (1930); *Japanese Journal of Physics* **7**, 31 (1931).

² T. Hori, *Zeits. f. Physik* **62**, 352 (1930); **71**, 478 (1931).

such that the piston could be advanced from outside the arc chamber. Thus potassium, contained in the cylinder, could be gradually extruded through the cap to keep a supply in the burning arc. A section of pressure tubing surrounded the piston shaft and its sleeve, soldered to the arc chamber, to prevent entrance of air. The shaft could be turned in the tubing. The upper electrode was of nickel or iron. Its shaft also entered the chamber through a sleeve, shaft and sleeve being surrounded by a section of tubing. The arc was struck by pressing the upper electrode against a coil spring.

Tank hydrogen was supplied continuously through a capillary tube. A pressure of about 20 cm of Hg was maintained, although the pressure did not seem to be a very critical factor in determining the intensity of the bands. Potential was supplied by a 500-volt d.c. generator and the current in the arc was held to about 3 amperes with series resistance. A single filling of potassium (about an ounce) could be made to last 3 or 4 hours. Exposures up to ten hours were taken.

Most of the analysis was made from photographs taken with an E-1 Hilger glass prism spectrograph. When the analysis was nearly completed a prism spectrograph fitted with a glass optical train (Hilger) consisting of a 60° prism, a 30° prism, and an achromatic lens of 3 meters focal length, in Littrow mounting, became available. This instrument was used to extend the spectrum above 5900A where the dispersion of the E-1 was insufficient to give satisfactory measurements. The larger instrument had a dispersion of 10A per mm at 6600A, equal to the dispersion of the E-1 at 5000A.

An attempt was made to photograph the KH spectrum in absorption. Potassium was heated, with hydrogen, in a length of iron tube, placed in a gas combustion furnace. The absorption spectrum was obtained but it was largely masked by other spectra. Below 4600A the spectrum of K₂ was prominent. Above 4800A the blue-green system of Na₂ (present as an impurity) extended up to the NaK bands falling just below the *D* lines of Na. Above the *D* lines the red system of Na₂ appeared. Between 4600A and 4800A, however, the spectrum of KH, corresponding exactly with the emission spectrum, could be observed.

ANALYSIS OF BAND SYSTEM

The KH spectrum is of the many-lined type; no heads or other regularities of structure are apparent on casual inspection. This is due to the fact that the heads of the bands almost coincide with the origins and to the overlapping of the bands. It is, therefore, not possible to make a vibrational analysis without first completing the rotational analysis, thus locating the band origins.

To carry out a rotational analysis, a beginning was made by picking out a branch of one of the stronger bands using the criterion that the second differences of the frequencies should be constant. This branch, being a strong one, could be followed through the origin and its character (*P* or *R*), as well as the rotational quantum numbers, determined. The combination differences,

$$\begin{aligned}\Delta_2 T' &= R(K'') - P(K'') \\ \Delta_2 T'' &= R(K'' - 1) - P(K'' + 1),\end{aligned}\quad (1)$$

were calculated for this band. Then bands in the same v' progression could be identified since they have the same value of $\Delta_2 T''$, while bands in the same v'' progression yielded identical values of $\Delta_2 T'$. Once the vibrational intervals were approximately determined the analysis proceeded rapidly. Often when the hunt for the correct combination differences did not give results promptly, a new start in the proper region with second differences disclosed the next band in a progression.

In this way 29 bands were located. The frequencies with quantum assignments are listed in Table VI at the end of this paper. Since about 85 percent of the lines appearing on the plates were assigned and since the remaining lines were mostly of very low intensity it is quite certain that the bands are of the simple two-branch type originating from a ${}^1\Sigma \rightarrow {}^1\Sigma$ transition. The system thus corresponds to the similar systems found for NaH and LiH, assigned to $p\sigma^1\Sigma \rightarrow s\sigma^1\Sigma$ transitions.

CALCULATION OF MOLECULAR CONSTANTS

The next step was the calculation of the rotational constants and the band origins. The combination differences were tabulated (Tables IV and V) and mean values taken where more than one value was obtained for a particular pair of rotational levels. Since the rotational energy of a molecule in a ${}^1\Sigma$ state is

$$T = B_v K(K + 1) + D_v K^2(K + 1)^2 + F_v K^3(K + 1)^3,$$

the combination differences can be expressed,

$$\begin{aligned}\Delta_2 T &= T(K + 1) - T(K - 1) \\ &= 4B_v(K + \frac{1}{2}) + 8D_v(K + \frac{1}{2})^3 + 12F_v(K + \frac{1}{2})^5\end{aligned}\quad (2)$$

where terms small in comparison with $F_v(K + 1/2)^5$ are dropped. B_v depends upon v according to the relation,

$$B_v = B_e - \alpha_e(v + \frac{1}{2}) + \gamma_e(v + \frac{1}{2})^2 \quad (3)$$

in which $B_e (= h/8\pi^2 I_e c)$ is the extrapolated value corresponding to the non-vibrating molecule. Theoretically D_v and F_v also depend on v but the accuracy of the present data did not warrant the calculation of this variation. Hence D_v was set equal to D_e and F_v equal to F_e .

A method of successive approximation was used to obtain B_v . First, the D and F terms of Eq. (2), which are relatively small, were neglected and approximate values of B_v obtained, using the measured combination differences from Tables IV and V. Then approximate values of D_e and F_e were calculated from the theoretical relations,

$$\begin{aligned}D_e &= -4B_e^2/w_e^2 \\ F_e &= (D_e^2/B_e)(2 - \alpha_e\omega_e/6B_e^2).\end{aligned}\quad (4)$$

ω_e was approximately known from the separations of corresponding lines in successive bands in a progression. α_e was assumed to be zero in this ap-

proximation. These values of D_e and F_e were then used in Eq. (2) to obtain the second approximation for B_v , the mean for several values of K being taken. The origins of the bands were then calculated from the equation,

$$\nu = \nu_0 + (B_v' + B_v'')M + (B_v' - B_v'' + D_e' - D_e'')M^2$$

in which ν_0 is the origin. For the R branch $M=K''+1$, for the P branch $M=-K''$. Here the F_e terms are omitted because they are inappreciable for the values of M (<15) used. From these calculated origins the vibrational intervals, ω_v , were determined and extrapolated to give ω_e . Then improved values of D_e and F_e were calculated from Eqs. (4) and the process described repeated to give a third approximation. This approximation was found to be sufficient, considering the accuracy of the data.

TABLE I. Band origins with values of ω_v interpolated.

$\nu'' \backslash \nu'$	0	1	2	3	4	Mean ω'_v	
0				16386.0	868.3	15517.7	
				259.5		259.5	259.5
1				16645.5	868.3	15777.2	
				266.5		266.6	266.6
2			17809.5	897.5	16912.0	868.2	16043.8
			272.7		271.8		272.2
3		19009.9	927.7	18082.2	898.4	17183.8	
		277.3		279.2			278.2
4		19287.2	925.8	18361.4			
		283.3		282.1			282.7
5	20527.4	956.9	19570.5	927.0	18643.5		
	287.8		288.9				288.3
6	20815.2	955.8	19859.4				
	290.5		(293.8)				290.5
7	21105.7	(952.5)	20153.2				
	291.5						291.5
8	21397.2						
	293.8						293.8
9	21691.0						
	293.0						293.0
10	21984.0						
	292.8						292.8
11	22276.8						
	291.6						291.6
12	22568.4						
	290.0						290.0
13	22858.4	955.1	21903.3				
			288.0				288.0
14			22191.3				
			284.4				284.4
15			22475.7				
			281.5				281.5
16			22757.2				
Mean ω''_v	955.9		926.8		898.0		868.3

In Table I the band origins are listed in square array with assignments of v' and v'' . The values of v'' are certainly correct but there is some doubt about v' . The correctness of the assignment of these quantum numbers will be discussed in the last section of the paper. The values of $\omega_{v'}$ and $\omega_{v''}$ also appear in Table I. In Fig. 1, $\omega_{v'}$ is plotted against v' , together with corresponding graphs for NaH and LiH, showing the anomalous increase in $\omega_{v'}$ with v' for low v' . $\omega_{v''}$ follows a normal course, decreasing linearly with increasing v'' . The values of $\omega_{v'}$ have been fitted with a power series in $(v+1/2)$

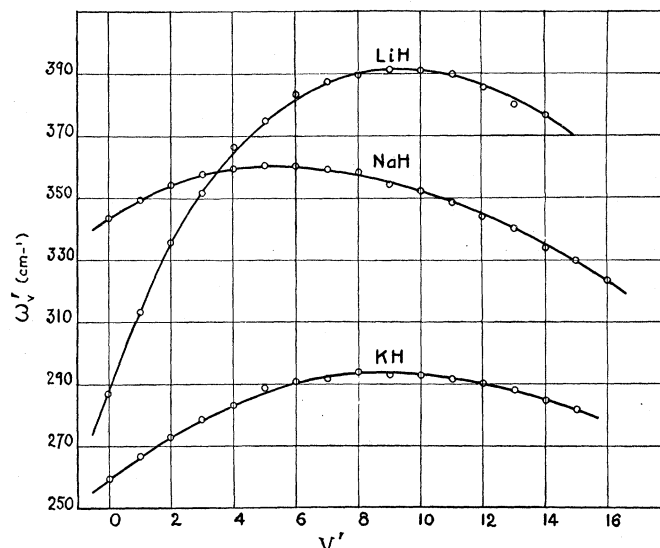


Fig. 1. Anomalous behavior of $\omega_{v'}$ in excited ${}^1\Sigma$ states of LiH, NaH, and KH.

by a least-squares calculation, with deviations, except one, less than 1 cm^{-1} . The result is incorporated in the following equation for the band origins,

$$\begin{aligned} \nu = & 19525.2 + [254.51(v' + \frac{1}{2}) + 3.26(v' + \frac{1}{2})^2 + 0.00725(v' + \frac{1}{2})^3 \\ & - 0.0105(v' + \frac{1}{2})^4 + 0.000273(v' + \frac{1}{2})^5] - [984.3(v'' + \frac{1}{2}) \\ & - 14.5(v'' + \frac{1}{2})^2]. \end{aligned}$$

The calculated values of $B_{v'}$ and $B_{v''}$ are listed in Table II. $B_{v'}$ parallels $\omega_{v'}$ in its anomalous behavior. It increases until $v'=6$ and then decreases.

TABLE II.

v	$B'_{v'}$	$B''_{v'}$	v	$B'_{v'}$	$B''_{v'}$	v	$B'_{v'}$	$B''_{v'}$
0	1.359	3.373	6	1.437		12	1.376	
1	1.385	3.292	7	1.432		13	1.360	
2	1.405	3.209	8	1.431		14	1.334	
3	1.422	3.122	9	1.416		15	1.323	
4	1.432	3.041	10	1.405		16	1.307	
5	1.438		11	1.391				

B_v'' decreases linearly with increasing v'' . The rotational and vibrational constants together with those of LiH and NaH, obtained respectively from Nakamura's and Hori's papers, are collected in Table III.

TABLE III. *Principal rotation and vibration constants.*

Constant	LiH	NaH	KH
I''_e	3.7×10^{-40}	5.65×10^{-40}	8.10×10^{-40} (g cm ²)
r''_e	1.6×10^{-8}	1.88×10^{-8}	2.24×10^{-8} (cm)
B''_e	7.38	4.896	3.415
α''_e	—	0.13	0.083
D''_e	—	-3.3×10^{-4}	-1.65×10^{-4}
F''_e	—	1.3×10^{-8}	1.5×10^{-8}
ω''_e	1395	1170.8	984.3
$x''\omega''_e$	22.7	18.9	14.5
I'_e	9.3×10^{-40}	14.66×10^{-40}	20.6×10^{-40} (g cm ²)
r'_e	2.5×10^{-8}	3.03×10^{-8}	3.58×10^{-8} (cm)
B'_e	3.00	1.887	1.344
α'_e	—	-0.028	-0.030
D'_e	—	-1.85×10^{-4}	-1.44×10^{-4}
F'_e	—	$\sim 0.8 \times 10^{-8}$	3.8×10^{-8}
ω'_e	272	335.24	254.5
$x'\omega'_e$	-9.61	-4.416	-3.26
Heat of dissociation $\begin{cases} D' \\ D'' \end{cases}$	$\begin{cases} 1.14 \\ 2.56 \end{cases}$	$\begin{cases} 1.47 \\ 2.24 \end{cases}$	$\begin{cases} 1.25 \text{ (volts)} \\ 2.06 \text{ (volts)} \end{cases}$

A satisfactory explanation of the peculiar behavior of the upper state has not been given. Following Nakamura's account of it in LiH, Weizel³ attempted to explain the anomaly as due to an uncoupling, as the rotation increases, of the orbital angular momentum l of the $p\sigma$ electron of the excited molecule. Such an effect would result in a calculated value of B_v less than the "true" B_v , the depression being greater for slower vibrations. Such an explanation is inadequate to account for the behavior of ω_v' . The positions of the origins should be independent of rotational uncoupling effects. It might be argued that since the origins were calculated from rotational data, the calculated positions of the origins does depend upon the uncoupling. If, however, one uses for ω_v' the frequency intervals between corresponding lines of successive bands—lines for which K'' is so small, say 2, that the rotation could scarcely affect it—one obtains a series of values of ω_v' inappreciably different from those obtained from the calculated origins. That is to say, the anomaly, at least for ω_v' , seems to be independent of any rotational uncoupling that may be present.

³ W. Weizel, Zeits. f. Physik 60, 599 (1930).

POTENTIAL ENERGY CURVES AND HEAT OF DISSOCIATION

Potential energy curves, based on the Kratzer form, are shown in Fig. 2. In the form used, the potential energy does not involve coefficients in the vibrational energy beyond the second ($x\omega_e$) nor coefficients in the expression for B_v (Eq. (3)) beyond α_e . Though ordinarily positive $x\omega_e$ and α_e are negative in the upper state of KH. This change tends to steepen the potential energy curve for $r > r_e$ and flatten it for $r < r_e$. For the ground state the potential energy curve was obtained from the Kratzer expression for r near r_e , while in the neighborhood of dissociation the Morse form was used.

The heat of dissociation of the lower state was calculated from the expression $D = \omega_e^2 / (4x\omega_e)$ since the vibrational energy in this state is accurately represented by $T^v = w_e(v + \frac{1}{2}) - x\omega_e(v + \frac{1}{2})^2$ with $\omega_e = 984.3$ and $x\omega_e = 14.5$. D is thus 2.06 volts.

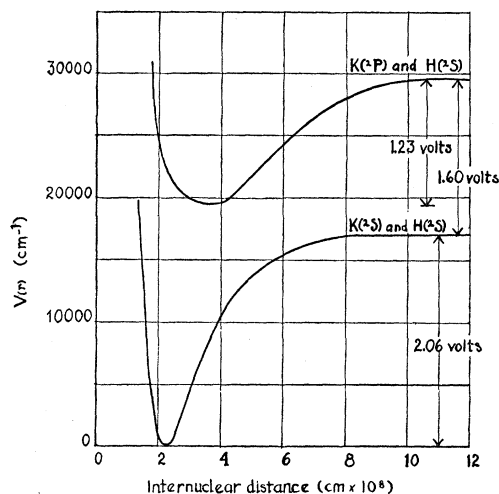


Fig. 2. Potential energy of normal and excited states of KH.

On account of the peculiar behavior of ω_v' the heat of dissociation of the upper state was determined by making use of the energy of the dissociated products. Rough extrapolation of the vibrational levels of the upper state indicated a heat of dissociation of about 1.5 volts. This requires that the atomic energy of the products of dissociation in the upper state be 1.8 volts greater than that of the products of the ground state. The resonance lines of potassium correspond to an excitation of 1.60 volts. Hence the products of dissociation in the upper state are normal hydrogen and potassium in the first excited state (2P). This atomic energy was added to D'' (2.06 volts) and the electronic energy of the excited molecular state (v_0) subtracted from the sum to give 1.25 volts for D' , the heat of dissociation in the upper state.

From the potential energy curves the Franck-Condon intensity diagram in Fig. 3 was drawn, using the improved form suggested by Loomis and Nusbaum.⁴ The theoretical locus of maximum intensity is shown by the

curve, the observed bands by small circles. The discrepancy at high frequencies is not surprising since the steep, uncertain, part of the energy curve of the upper state is involved.

ASSIGNMENT OF v' AND v'' . ISOTOPE EFFECT

The assignment of v'' is certainly correct since a thorough search on emission and, more important, on absorption photographs disclosed no bands of a lower progression than the one for which v'' was set equal to zero. As to the upper state we suggested in a preliminary report⁵ that the bands now marked $v' = 4$ belonged to the state for which $v' = 0$. Improvements in technique enabled us to extend the spectrum to the red four vibrational intervals of the upper state. In the progression for which we now put $v' = 0$, there are only two bands, (0, 3) and (0, 4). The evidence for the present assignment is

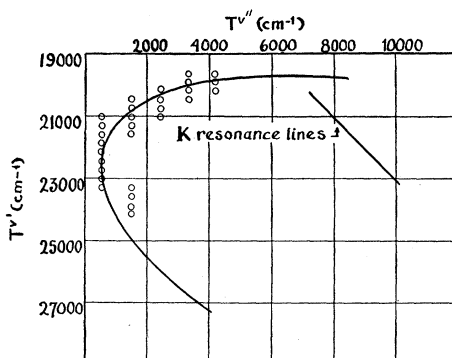


Fig. 3. Intensity diagram for KH. Circles are observed band origins.
Curve is theoretical locus of maximum intensity.

first, that no bands assignable to a lower v' could be found even though the bands in this region (6100Å–6500Å) were well developed in the long exposures and, second, that the assignment fits well with the Franck-Condon curve, which is most reliable in this region. Additional evidence was sought through the isotope effect. The heavier isotope of potassium, of mass 41, is present in the ratio of about 1 to 20. No lines of $K^{41}H$ could be found in the emission photographs. In the absorption photographs, limited to the region 4600–4800Å, faint lines accompanied the intense lines in about the estimated positions. Measurements of the isotope shifts (about 1–2 cm⁻¹) made on two plates, were not sufficiently accurate to fix with certainty the v' assignment. Averages of calculated and measured values indicate that the assignment is about right, but may still be too high by one. Such a change would make little difference in any of the molecular constants listed.

⁴ F. W. Loomis and R. E. Nussbaum, Phys. Rev. **38**, 1447 (1931).

⁵ G. M. Almy and C. D. Hause, Phys. Rev. **39**, 178 (1932).

TABLE IV. (Continued). $R(K-1) - P(K+1) = T''(K+1) - T''(K-1) = \Delta_2 T''(K)$.

K	$v'=3$	$v'=4$	$v'=5$	$v'=6$	$v'=7$	$v'=13$	$v'=14$	$v'=15$	$v'=16$	Mean
5	70.2	70.2	(68.5)	(74.2)	(67.7)	72.5		71.3	71.9	71.5
6	83.5	84.4	(82.3)	(81.1)	84.8	85.7	84.4	84.6	83.9	84.5
7	99.3	98.4	(95.5)	98.5	100.6	98.1	97.7	98.4	99.4	98.8
8	(113.5)	110.6	111.5	111.7	(114.4)	110.1	111.2	111.2	(109.9)	110.0
9	—	123.7	125.3	124.0	124.0	123.1	124.3	124.2	124.6	124.1
10	135.1	137.0	136.1	138.1	138.7	136.9	135.5	135.9	137.4	136.7
11	150.2	149.7	149.9	149.1	150.7	148.5	149.0	149.6	150.3	149.6
12	161.5	162.3	161.8	161.9	(165.6)	162.8	161.3	162.8	162.2	162.1
13	175.0	174.0	175.5	—	174.6	174.3	174.4	174.4	173.5	174.4
14	—	186.6	187.7	187.6	186.7	186.7	186.8	186.9	187.1	187.0
15	199.3	200.5	199.2	198.6	200.9	199.8	199.8	199.9	199.7	199.7
16	212.4	211.0	211.5	210.5	212.7	211.4	211.7	211.7	211.3	211.6
17	222.8	223.9	223.2	223.3	223.0	223.3	221.7	221.7	223.0	223.0
18	235.6	236.9	235.5	235.5	235.9	234.2	235.3	235.3	234.8	235.5
19	245.7	—	247.5	245.6	248.5	245.8	247.6	247.6	246.5	246.8
20	258.5	260.2	259.4	259.2	259.5	—	258.9	258.9	258.4	259.1
21	271.5	270.3	270.3	270.9	270.7	270.7	271.1	271.1	270.8	270.8
22	284.4	282.2	—	292.1	282.2	—	282.6	282.6	282.8	282.8
23	—	293.8	292.5	292.1	293.3	—	292.3	292.3	292.8	292.8
24	—	304.4	303.9	304.0	303.0	—	303.0	303.0	303.8	303.8
25	—	—	313.7	314.8	314.1	—	314.1	314.1	314.2	314.2
26	—	—	—	326.0	326.0	—	326.0	326.0	326.0	326.0
27	—	—	—	336.2	335.6	—	335.6	335.6	335.9	335.9
28	—	—	—	346.2	345.9	—	345.9	345.9	346.0	346.0
29	—	—	—	356.2	354.4	—	354.4	354.4	355.3	355.3
30	—	—	—	366.5	—	—	—	—	366.5	366.5

TABLE V. (Continued). $R(K) - P(K) = T'(K+1) - T'(K-1) = \Delta_2 T'(K)$.

K	$v''=0$	$v''=7$ $v''=1$	Mean	$v''=8$ $v''=0$	$v''=9$ $v''=0$	$v''=10$ $v''=0$	$v''=11$ $v''=0$	$v''=12$ $v''=0$	$v''=13$ $v''=0$	Mean
1	14.6		14.6	8.3	(10.0)	(10.2)	16.1	(7.3)	13.5	13.5
2	20.0		20.0	14.2	13.7	14.5	—	13.3	18.5	18.5
3	24.9		24.9	19.7	19.0	20.0	25.5	18.3	24.3	24.3
4	31.6		31.6	25.0	25.2	24.5	31.9	24.4	29.0	28.5
5	37.1		36.7	30.9	30.3	30.2	37.8	29.2	35.2	34.6
6	42.2	36.3	39.8	37.4	36.1	35.9	42.0	34.4	39.4	39.1
7	47.6	41.5	44.6	42.5	41.6	41.3	46.5	40.4	44.6	44.2
8	53.6	(50.3)	52.0	46.8	46.8	46.4	51.8	45.5	50.8	50.8
9	58.2	(57.7)	58.0	52.5	52.3	52.2	56.6	51.2	54.9	54.9
10	63.6	(56.9)	60.3	58.7	57.6	57.2	62.7	61.0	60.3	60.4
11	68.8	63.5	66.2	63.6	63.0	61.8	66.9	65.9	64.7	65.1
12	74.2	66.1	70.2	68.5	68.4	67.5	71.9	71.4	70.5	70.3
13	79.5	75.1	77.3	74.0	72.9	73.0	77.2	75.7	75.0	75.5
14	85.5	80.9	83.2	78.9	78.6	77.9	81.8	81.3	79.7	79.9
15	89.5	86.2	87.9	84.7	83.6	81.9	87.3	86.2	84.9	84.5
16	94.1	89.8	92.0	89.2	88.5	87.9	91.5	90.5	89.6	89.6
17	99.9	94.5	97.2	94.3	93.5	92.8	96.3	94.7	94.0	94.0
18	104.8	99.4	102.1	99.7	98.8	97.6	100.7	99.5	99.1	99.1
19	108.7	104.8	106.8	103.6	103.0	102.1	106.0	104.6	103.5	103.1
20	114.0	109.4	111.7	109.0	107.9	106.1	109.5	108.2	106.7	106.7
21	115.8	113.7	114.8	112.5	112.1	111.4	113.2	110.6	111.9	111.9
22	119.3	119.4	119.4	118.7	116.8	115.5	117.6	117.9	116.5	116.5
23		122.4	120.8	122.6	120.2	120.1	123.0	123.2	120.2	120.2
24		126.4	126.4	127.5	124.6	124.1	126.4	126.4		
25		130.7	130.7	132.7	128.4	129.5	128.5	130.5		
26		133.3	133.3		132.3	132.9	131.6	(134.1)		
27		138.4	138.4			138.4	132.5	(136.6)		
28		140.6	140.6							

TABLE V. (Continued). $R(K) - P(K) = T'(K+1) - T'(K-1) = \Delta_2 T'(K)$.

K	$\frac{v'=14}{v''=1}$	$\frac{v'=15}{v''=1}$	$\frac{v'=16}{v''=1}$
3		16.6	22.6
4		23.8	26.1
5		29.0	33.2
6		33.6	37.1
7		38.0	44.0
8		44.2	47.8
9		48.7	53.4
10		54.1	58.6
11		58.4	63.0
12		63.6	67.3
13		68.8	72.4
14		73.4	77.0
15		78.2	80.9
16		83.0	85.5
17		87.5	89.4
18		90.5	(93.9)
19		96.2	(98.6)
20		101.3	(101.3)
21		104.9	
22		108.3	

TABLE VI. Wave numbers and quantum numbers of all assigned lines. Vibrational quantum numbers and band origin head each band. A line marked with an asterisk is assigned at least twice. Under intensity, d = diffuse, db = probably double.

K	I	R	(5,0)	I	P	(6,0)	R	I	P	(7,0)	R	I	P	(21,105.73)	I	P
0																
1	6d	20,529.2*				5	20,819.0*			3	21,108.4*					
2	0	525.3		1	20,511.6	5	819.0*		20,808.4	3	108.4*				0	089.5
3	1	516.0		1	497.3*	1	813.0		799.1	2	104.0				1	074.6
4	1	503.1		3d	479.1*	1	804.4		783.4*	3	094.7				1	056.7
5	1	487.0		0	455.7	4	790.9*		766.3	6	081.6*				2	034.3
6	1	466.1*		1	429.6	2	774.7		743.6	3d	066.0*				2	007.6*
7	3	442.0		1	399.8*	2	754.0		716.7*	6	044.6*				5	20,977.5
8	1	413.3		2d	366.0	2	729.7		686.8*	3	019.8				3	20,943.8
9	2	381.5		2	327.8	3	701.2		653.9*	3	20,991.4				3	905.5*
10	2	345.1		3	286.9	2	669.0		615.5	4	959.1				4d	864.5
11	2	303.2		1	240.7*	2	632.8		574.1	4	922.7				3	819.0*
12	1	261.4		3	192.7*	1	592.7		529.2*	3	822.6				5	769.5
13	2d	210.7		4		2	549.0		479.1*	4	838.3*				3	710.7*
14	0					2	501.3		526.8	4	790.9*				4	659.4
15						2	449.6*		368.9*	2	739.0				3	599.0
16						2	394.3*		309.6	2d	684.5*				2	534.5
17						3d	335.2		245.2	5d	624.0*				2	466.1*
18						1	271.7*		177.6*	3	560.2				3	394.3*
19						0	205.6		105.9	3d	494.2				3d	319.2
20						10-K	134.7		30.4	1	423.9				2	240.7
21						0	60.6*		19,951.8	2	271.7*				3	157.7
22									869.7	1	187.1				1	071.4*
23										1d	105.9*				1	19,982.1

TABLE VI. (Continued).

K	I	R	I	P	I	R	I	P	I	R	I	P
0												
1	1	21,400.4*		21,392.0	3	21,694.3*		21,684.2	2	21,987.9*		21,977.7*
2	4	400.4*	1d	381.8	3	694.3*	2	675.3	2	987.9*	2d	968.4
3	1	396.0*	1	367.2	2	689.0	1d	660.7	3d	982.9*	1	953.1*
4	2	386.9	3	348.6*	2	679.7	1	641.5	1	973.0	3	935.3*
5	2	373.6	3	326.4	2	666.7	2d	619.2*	2	959.7*	5	912.5
6	3	357.2	3	299.5	3	649.6*	3d	592.7	3	942.7	2	885.5
7	6	336.9*	6	269.1	3	628.8	2	562.4	3	921.5	3	855.3*
8	5	311.5*	4d	235.6	3	604.0*	3	528.3*	3	896.6*	4	821.0
9	4d	282.4	4	197.7	2	575.1	4	490.2	3	867.4	3	782.6*
10	6	250.3*	4	155.8*	4	542.5	3	448.0	3	834.3*	4	740.2
11	4d	214.5*	4	110.0	3	505.7	3	402.2	3	797.4	3	694.3*
12	5	173.6	3	060.8	3	465.2	3	352.6	3d	756.2*	3	644.1
13	4d	129.2	3	007.6	3	421.0*	3	299.5*	3	711.6	3	590.3
14	6	081.6*	5	20,950.5	5	372.4	6	241.5	4	663.4*	2	532.7
15	4	029.3	4	889.6	4d	320.2*	4	180.7	3	610.6	2	471.4
16	4d	20,9743*	3	825.0	5	264.3*	4	115.7	4dd	553.3*	3	405.9
17	4	914.2	3	756.0	3	204.2	3	047.1	3	429.7	6	336.9*
18	2	850.8	2	684.5	3	140.6	3	20,974.3*	3	361.9	5	264.3*
19	4	783.4*	5d	609.5	3	073.1	4d	899.1	3	290.5*	3	188.4
20	2	713.1	2	529.2	3	002.1	3	819.0	3	214.5*	3	108.4*
21	2	638.2	6d	447.6	3	20,927.0	5	736.4	4d	135.8	3	024.7
22	3d	460.2*	2	360.4	2	848.5	2	649.5	2	053.0	2	20,937.5
23	3d	479.1*	2	271.7*	3	766.3*	2	560.2*	2	20,966.8*	2	846.7
24	3d	394.3*	2	177.6*	2	680.4	3d	466.1*	2	876.6	2	752.5
25	1	305.1	2	080.8	1	590.6	3	368.9*	3	783.4*	3	653.9*
26	0	213.5	2	19,979.9	1	497.3*	2d	267.5	4	686.8*	1	553.0
27	1		1	876.4	2d	399.8*	1	162.5	3	586.0	2	449.6*
28	0d								3d		2	340.9*

TABLE VI. (Continued).

K	I	R	I	P	I	R	I	P	I	R	I	P
		(11,0)	(22,276.80)			(12,0)	(22,568.44)			(13,0)	(22,858.44)	
0												
1	3	22,275.2*			2	22,570.8*						22,851.5
2				22,259.1*	2	570.8*						842.1
3				243.4*	2	566.3*						827.7
4	1	250.3		224.8	2	556.4*						808.8
5	1	233.1		201.2*	2	543.1						786.0
6	3	213.6		175.8	2	525.3*						758.3
7	1	188.1*		146.1*	1d	503.8						728.0
8	2	158.9		112.4	2	479.0*						692.8*
9	3	125.6*		074.2*	2	449.2*						653.3
10	2	088.4		031.8	3	415.9*						610.3
11	4	047.1*		21,985.3	3	377.9*						563.5*
12	3	002.2		935.3*	3	336.2*						512.9*
13	3	21,955.1*		881.1*	2	290.7						457.2
14	3	900.3*		823.0	2	241.6						398.6
15	2	843.0		761.2*	5	188.1*						336.2*
16	4	782.6*		695.3	2	130.7						269.7
17	2	718.0*		626.4*	3	069.1*						199.3
18	3	649.6		553.3*	3	004.3*						125.6*
19	2	577.3		476.6	3d	21,935.3*						047.1*
20	3d	502.0*		396.0*	2d	862.3*						21,965.6*
21	4d	421.0*		311.5*	3d	786.4*						881.1*
22	6	336.9*		223.7	3d	619.2*						791.3
23	6	250.3*		132.6	3	534.8						698.9
24	2	160.9		037.8	1	443.4						602.5
25	3d	066.0*		20,939.5	3	348.6*						502.0*
26	1	20,966.8*		838.3*	6	250.3*						400.4*
27	2	864.3*		732.7	2	147.7*						292.9
28	2	756.6*		624.0*	1	042.0						

TABLE VI. (Continued).

K	(3, 1)	R	I	P	(4, 1)	R	I	P	(5, 1)	R	I	P
1						19, 290.9		19, 272.0		19, 544.9		19, 499.2*
2					0	284.4	2d	256.3				476.4
3		18, 996.8	0	18, 977.5	0	276.4*	1db	239.7*	1d	529.3	1	447.0
4	1	983.1*	2	938.7*	2d	263.8	1d	216.4	1	510.4*	1	414.9
5	1db	969.1	2	912.9*	1	247.6*	3	193.6*	1	489.3	2	377.8
6	2d	951.3*	1	912.9*	1d	229.0	1d	163.2	2	463.1	1	337.8
7	2	928.7*	2db	885.6*	2d	205.1	1	130.6	1d	431.2*	2db	295.1
8	2	898.3	3d	852.3*	3	178.0*	1	094.5	2	397.5	1d	247.6*
9	2	868.8*	2	815.2	2	147.9	3	054.3*	2	359.6	2	197.8
10	2	833.7*	2	733.7*	3	113.8*	1	18, 964.1	2	318.3*	3db	142.8
11	2d	795.4*	2db	733.7*	2	075.2	1	010.9	3	272.0*	2	084.3
12	2	753.1	2	683.5	1	033.2	2	18, 990.6	2	223.1	2	023.9
13		K	2	633.9	2	18, 987.4*	2	18, 990.6	2	113.8*	2	18, 959.0*
14	1	657.4	2	578.1	2	938.7*	2	605.3*	2	054.3	2	890.6*
15	2	605.3*	2	520.1	2	885.6*	2	532.7*	2	923.5	2	818.8
16	2d	546.9*	3d	458.1*	2db	829.2	2	458.1*	3d	852.3*	2	743.1
17	2	487.8*	1	392.9	1	769.6	2	379.3*	3d	K	2	664.1
18	2d	421.7*	2	324.1*	1	K	2	296.6*	1	700.2	2	582.0
19	2d	354.8	1d	252.2	2	638.5	2	209.9*	1db	618.5	2	496.4
20	1	284.2*	2	176.0*	2	566.9*	3d	120.4*	2	532.7*	3	407.7*
21	4	209.9*	2	096.3*	2	492.1*	3	027.8*	2		1	314.6*
22	0	133.7*	2db	012.7*	1	414.2	1	067.3	1		1	219.0
23	1d	051.0	2db	17, 925.5*	1d	332.2*	4	160.0*	2		4	120.4*
24					3	248.1	4	17, 972.3				018.5
25					1	160.0*	3db					
26					1	067.3						
27					2db	17, 972.3						
28					1d	873.5						
29					3d	771.8*						
30					1	665.4						

TABLE VI. (Continued).

K	I	R	I	P	I	R	I	P	I	R	I	P
		(14, 1)	(22, 191.26)		(15, 1)	(22, 475.69)		(16, 1)	(22, 757.19)			
3				22, 142.2	0	22, 461.8	1	22, 445.0		22, 731.5	0	22, 708.9
4				119.7	3*	449.2	1	426.8		713.1	1	686.9
5		22, 147.9		127.3	2	432.7	2	403.7*		692.8*	0	659.6
6		102.7		092.8	3d	411.5	3	377.9*		666.3	0	629.1
7		074.2*		063.6	1	386.4	2d	348.0		637.4	0	593.4
8		041.0		029.5	2	357.3	1	313.1		604.2	1d	556.4
9		004.3*		21, 991.4	2	324.0	3d	275.3*		566.3	2	512.9*
10				950.0	2	287.2	1	233.1		525.3	2	466.8
11		21, 963.8		905.5	3d	246.5	4	188.1*		479.0	1d	415.9*
12		919.5*		855.3*	2	201.2*	1	137.5		430.5	3d	363.2
13		871.0		802.6	2	152.5	2d	083.7		320.4	1	305.5
14		819.0		744.9	2	100.2	2	026.7		259.1	3	243.4
15		762.8*		684.2*	1	043.8	2	21, 965.6*		194.6	0	178.2
16				619.2*	3d	21, 983.3*	3	900.3*		125.6*	1	109.1
17					2	919.5*	2	832.0		055.7	3	036.1
18					0	851.6	3	761.2*		21, 977.7*	1	21, 959.7*
19					2	780.4	2	684.2*		896.6*	2	795.3
20					3d	705.3*	3	604.0			1	
21					3	626.4*	2	521.5			1	
22						542.5*	1	434.2			3	
23							2	343.8			6	
24							6	250.3*			4	
25							4	155.8*				

TABLE VI. (Continued).

K	I	R	I	P	I	R	I	P	I	R	I	P
	(2, 2)	(17, 809.50)	(3, 2)	(18, 08.25)	(4, 2)	(18, 361.27)						
4	3	17,748.8*	1d	18,045.5	1d	18,338.9	3	18,314.6*				
5	3	730.1	3d	027.8*	3d	324.1*	1	296.6*				
6	1	704.2	2d	003.2*	2d	305.8*	1d	272.7				
7	3	656.8*	3	17,979.5*	3	284.2*	3	242.4*				
8	1	674.7	3	949.6*	2d	258.7	4	209.9*				
9	3	639.6*	3	916.0	2	229.7	2	176.0*				
10	2d	604.6*	2	879.2	2	196.1	1	138.0				
11	3	541.4	2	839.0	3	160.0*	2	096.3*				
12	2d	565.3	1	796.5	3d	120.4*	2	051.0*				
13	2d	520.2	3	748.8*	1d	077.0	1d	003.2*				
14	1d	472.5	3	698.0	3	027.8*	2d	003.2*				
15	2	421.3	3d	338.5	3	669.8	3	17,949.6*				
16	1	366.7	3d	338.5	2	614.4	2	895.5*				
17	2d	308.4	1d	279.0	2d	555.0	3d	835.0				
18	3d	246.4*	2	215.2	2d	491.7*	3	771.8*				
19	1	182.1	2	149.2	3	426.4	2	707.5				
20	1	112.7*	2	079.1	2d	356.4	2d	639.6*				
21	2	040.0*	2	006.4*	3d	393.4*	3	—				
22	0d	Na	3d	16,928.9*	2	321.0	4	491.7*				
23	2	16,886.0*	2d	847.4	3	246.4*	2	412.6				
24	3	804.0	3	765.1*	2	679.6*	2	330.4				
25	1		1	589.5			3d	246.4*				

TABLE VI. (Continued).

K	I	R	I	P	I	R	I	P	I	R	I	P
		(5, 2)	(18, 643.48)		(0, 3)	(16, 386.0)		(1, 3)	(16, 645.50)			
2	2	18,566.9*	2	18,492.1*	1	16,336.6	1	1d	16,646.0	0	16,631.8*	
3	1	540.1	1	458.1*	1db	310.6	1	2d	637.3*	1	620.3*	
4	1d	512.5	3d	421.7*	1	282.6	2	1d	625.1*	2	605.5	
5	1	480.7	2d	379.3*	0d	254.3	0	1d	608.9	1	585.6*	
6	1	445.3	3	332.2*	1	221.4	2	1	589.5*	2d	556.7	
7	1	404.2	1d	287.2	2	189.5*	0	2	569.7	1	527.1	
8	1	361.5	1	232.9	2	143.1*	1	1d	544.2*	1	495.9	
9	2d	314.6*	1	181.8	1	99.7	0	2	516.7	1	464.2	
10	3	263.8	1	120.4*	1	054.6	1	1d	484.0*	1	426.9	
11	4	209.9*	1	152.7	0	031.1	2	2d	448.8	1	386.2	
12	2	152.7	4	120.4*	2	024.0*	1	1d	409.0	3	342.8	
13	3d	91.8*	3d	89.4*	1	003.5*	2	2	366.8	2d	295.1	
14	3d	027.8*	2db	851.9	0	15,950.1*	2d	2	320.6*	2	243.8*	
15	1	890.4	2	17,991.2*	0	865.5	3	2	271.7	2	189.5*	
16	3	816.1*	2	925.5*	4db	835.9*	1	1	218.8	2db	133.0	
17	2	738.2	4	851.9	1	774.8*	1	1	161.3	3	069.9*	
18	2	656.8*	3d	851.9	0		0d	2	102.6	1	007.0	
19	2	574.0	2db					2	039.8	3	15,939.3*	
20	2	485.5	2					2	15,973.1*	1	15,868.3	
21	3d	393.4*	2					1	903.4*	0	795.7	
22	1		2					2	830.8*	2	716.6	
23	3		2					3d	754.4*	2	635.8*	
24	2		2					2	673.6	2	552.9*	
25	2		2					1	590.6*	3d		
26	2		2					2	503.7			
27	3d		3d					3				

