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The ν_2 Band of CHD_3; Ground State Parameters for CHD_3 from Combination Differences*†

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ν_2 of CHD_3

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ABSTRACT

The ν_2 fundamental band of CHD_3, centered near 2143 cm^{-1}, has been recorded at a resolution of 0.015-0.025 cm^{-1}. Analysis of ground state combination differences has yielded well-determined values for the ground state molecular parameters B_o, D_o^J, D_o^{JK}, H_o^J, H_o^{JK}, and H_o^{KJ} for CHD_3. These parameters have been used in the determination of the molecular parameters α_2^B, $(\alpha_2^A - \alpha_2^B)$, β_2^K, β_2^{JK} and β_2^J for ν_2.

Background

Triply deuterated methane is an oblate ($I_z > I_x = I_y$) symmetric top belonging to the C_{3v} Group. Therefore, C_o is smaller than B_o and both are large. Wilmhurst and Bernstein (1) have studied CHD_3 in the 900 - 3500 cm^{-1} region under low resolution. Rea and Thompson (2) have analyzed ν_2 and identified up to ^QP_K (12), ^QQ_K (18), and ^QR_K (11), but were unable to resolve the K structure. Blass and Edwards (3) have used data from $\nu_1+\nu_2$ obtained at 0.05 cm^{-1} resolution (with resolved K structure) to determine the ground state constants from ground state combination differences. From 54 combination differences they obtained the values: $B_o = 3.2795$ cm^{-1}, $D_o^{JK} = -4.0 \times 10^{-5}$ cm^{-1}, and $D_o^J = 5.2 \times 10^{-5}$ cm^{-1}.

The fundamental ν_2 is a parallel type band corresponding to the CD_3 symmetric stretching mode. Centered near 2143 cm^{-1}, it is bordered on the high-frequency side by the perpendicular band ν_4.

Experimental

The spectra were taken with 4 Torr pressure of CHD_3 in a 12m path at ambient temperature. The CHD_3 was obtained from Merck, Sharp, and Dohme and used without further purification. The spectra were recorded using the five meter Littrow instrument and a Bausch and Lomb 20 x 40cm, 31.6/mm echelle in eleventh and twelfth orders. The slit width was varied during the scans to keep the recorded signal level high. The data were recorded digitally at a rate of approximately 2.8 cm^{-1}/hr and measured from the machine readable

records. Resolution in the recorded spectra was between 0.015 cm^{-1} and 0.025 cm^{-1}.

Calibration

Calibration was accomplished using the 1-0 carbon monoxide band occurring in eleventh and twelfth orders, in the same region as ν_2. Some CO lines were present in the spectra due to a small impurity in the sample. The high and low wavenumber regions of the band were calibrated with additional CO added to the sample, and certain calibration lines were inserted by changing grating orders.

Twenty-two calibration lines were used in the region 1978-2103 cm^{-1} in eleventh order and thirty-five lines were used in the region 2082-2271 cm^{-1} in twelfth order. The standard deviations of the calibration fits were 0.0031 cm^{-1} for eleventh order and 0.0032 cm^{-1} for twelfth order.

Assignment and Weighting

For J>18 the P side was too low in intensity to be observed. This was also true in the Q region for J>22. The R side overlaps with ν_4, which limited the identifiable lines to J<13.

The transition assignment of lines up to $^{Q}P_{K}(11)$, $^{Q}Q_{K}(10)$, and $^{Q}R_{K}(9)$ were made from direct inspection of the spectra, since the structures of the K series were easily recognizable. Above these J values there are obvious intensity and frequency perturbations.

The $^{Q}Q_{J}(J)$ lines for high J could still be identified,

however, since these are the stronger lines in the Q region. The band was fitted to the transition frequency expression with a least squares regression program (4,5), and unknown transition frequencies were calculated. On the basis of these calculations and the relative line intensities, additional high J lines in the Q region were identified.

The high J assignments in the P and R regions were made using ground state combination differences. The combination differences were calculated using values for the rotational constants B_o, D_o^J and D_o^{JK} given by Blass and Edwards (3). By adding the combination differences to the frequencies of identified transitions in the Q region, the frequencies of transitions in the P and R regions with the same upper state were found (the transitions $^{Q}P_{K}(J+1)$, $^{Q}Q_{K}(J)$, and $^{Q}R_{K}(J-1)$ have a common upper state). These calculated frequencies were then used to identify P and R lines.

Each line was assigned a relative weight between 0.1 and 1.0 by inspection, on the basis of the line width $\Delta\nu$. The relation

$$\text{weight} \propto \frac{1}{(\Delta\nu)^2} \tag{1}$$

was applied approximately.

The Q region is shown in Figure 1, with assigned lines indicated. The perturbations of intensity and frequency in the

high J lines can be clearly seen, and the most striking feature is the complete absence of the low K, J = 11 lines. For J>10 the perturbations seem to be most pronounced at the lower K values, and the J=K lines are prominent and close to their expected positions. In most cases, if a $^{Q}Q_{K}(J)$ transition was perturbed the apparent intensity of the $^{Q}P_{K}(J+1)$ and $^{Q}R_{K}(J-1)$ transitions (with the same upper state) were perturbed in a similar manner.

As an example of the structure of the K series (for a given J) in the P and R regions of the band, Figure 2 shows the set of lines $^{Q}P_{K}(10)$. The K^2 dependence of the line positions is evident.

Tables I,II, and III list the observed transitions in the P, Q, and R regions, respectively, the give the frequency and relative weight of each transition.

Ground State Parameters from Measured Combination Differences

The ground state combination differences (G.S.C.D.) were found from the differences between transition frequencies represented by

$$\text{G.S.C.D. } (\Delta J_1 \Delta J_2 K, J) = {}^{Q}\Delta J_{1K}(J-\Delta J_1) - {}^{Q}\Delta J_{2K}(J-\Delta J_2) \qquad (2)$$

where J corresponds to the upper state. A weight for each G.S.C.D. was calculated from the weights of the two transitions using the relation

$$W_{\text{G.S.C.D.}} = \left[\frac{1}{\sqrt{W_1}} + \frac{1}{\sqrt{W_2}}\right]^{-2} . \qquad (3)$$

The weighted G.S.C.D.'s were used to find the ground state parameters B_o, D_o^J, D_o^{JK}, H_o^J, H_o^{JK}, and H_o^{KJ} as described by Blass (6) and Blass and Edwards (7). A least-squares regression analysis program was used to fit the G.S.C.D.'s to the expression given in (7). The program was allowed to delete G.S.C.D.'s with weighted residuals greater than 0.020 cm^{-1} and was allowed to omit insignificant terms from the regression model. The final regression fitted 238 observed combination differences with a standard deviation of 0.0073 cm^{-1} The resulting ground state parameters are given in Table IV. Table V provides a comparison with results of previous work on this molecule. To the knowledge of this author, no determination of H_o^J, H_o^{JK}, or H_o^{KJ} had been made for CHD_3 before this work. The confidence intervals for the coefficients obtained here are much narrower than those previously obtained.

Molecular Parameters for ν_2

A least-squares regression analysis was performed on the observed transitions in ν_2, using the transition frequency expression through fourth order (6, 12, 13) as the regression model. The regression procedure is described by Kurlat (4) and Hafford (5). The regression program uses the stepwise algorithm of Efroymson (14) and parameters not found to be statistically significant are effectively constrained to zero. Since the model equation used is a minimum

correlation model (15) there is no question of constraining, say, upper state distortion constants to be equal to the ground state values since upper state parameters do not explicitly occur in the model. For example, the minimum correlation model determines D_o^J and β_2^J rather than the more highly correlated parameters D_o^J and D_2^J. The rotational coefficients determined from G.S.C.D.'s (previous section) were fixed. Transitions with weighted residuals greater than 0.015 cm^{-1} were deleted at each regression. The final regression fitted 251 transitions with a standard deviation of 0.0082 cm^{-1}. Table VI lists the determined molecular parameters for ν_2.

Conclusion

Highly precise ground state parameters have been determined for CHD_3 including H_o^J, H_o^{JK} and H_o^{KJ}. Using a minimum correlation transition frequency model and a stepwise regression algorithm, all statistically significant remaining parameters through fourth order have been determined. Parameters not shown in Tables IV and VI were not found to significantly reduce the standard deviation of the regression (4-6, 8).

The character of a perturbation occurring for high J levels is briefly described and sufficient information is contained in Tables I-IV, VI for the interested reader to further study this resonance. Additional work is in progress on the resonance and any further comment would be premature.

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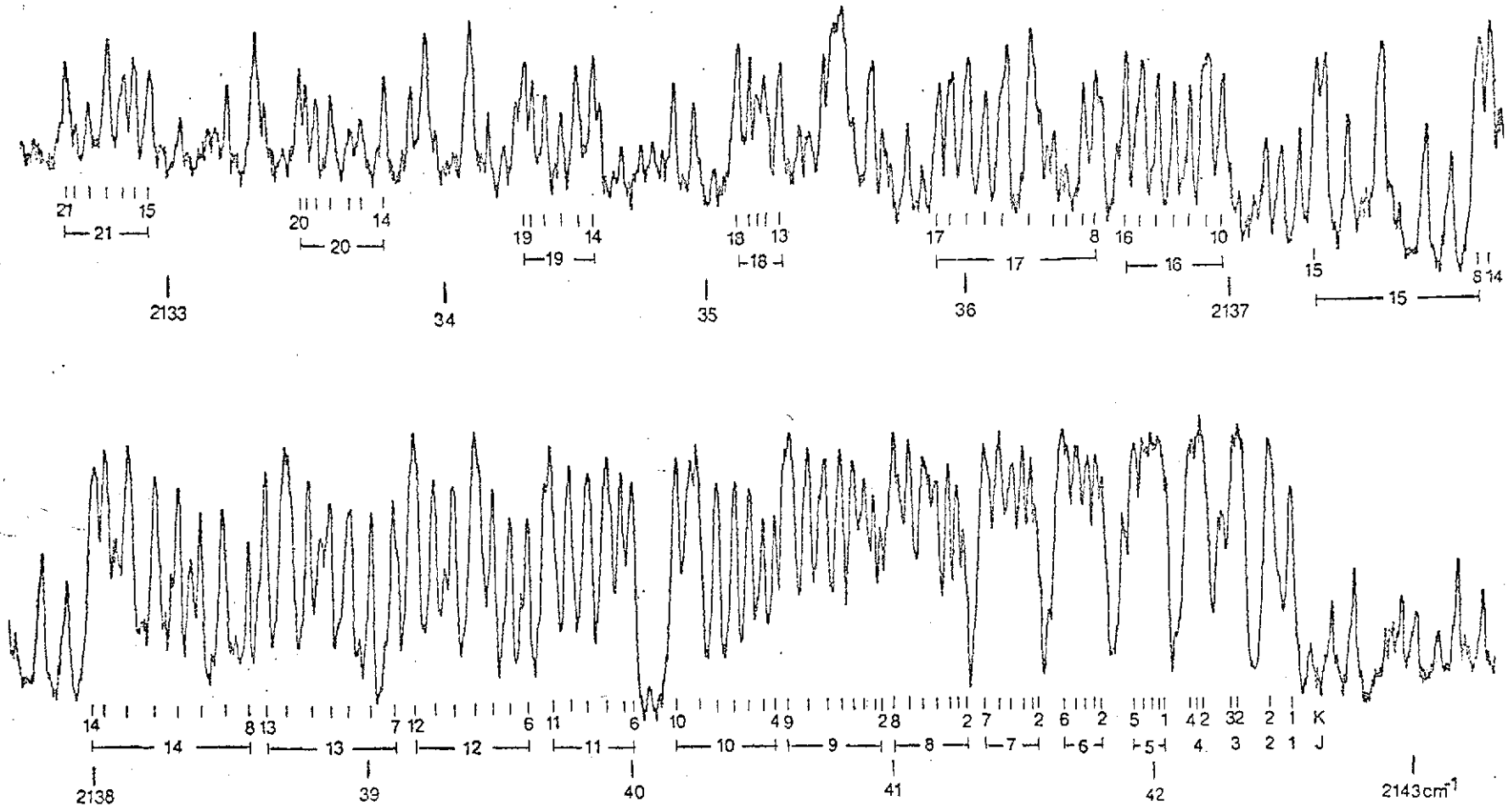
Figure 1. $^{Q}Q_{K}(J)$ transitions in ν_2 of CHD_3.

Figure 2. $^{Q}P_{K}(10)$ transitions in ν_2 of CHD_3.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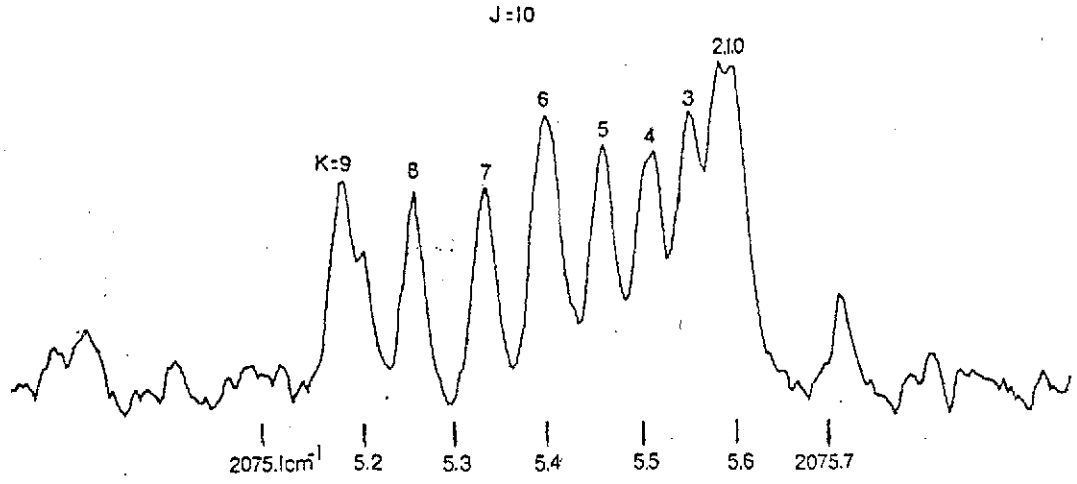
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TABLE I

Observed $^{Q}P_{K}(J)$ Transitions in ν_2 of CHD_3

J	K	Freq.[a]	Wt.	J	K	Freq.	Wt.	J	K	Freq.	Wt.
18	17	2018.5962	1.0	13	10	2054.4077	0.7	9	6	2082.2263	1.0
18	16	2018.7180	0.2	13	9	2054.5032	1.0	9	5	2082.2830	1.0
18	15	2018.8105	0.3	13	8	2054.5938	1.0	9	4	2082.3335	0.5
18	14	2018.9084	0.2	13	7	2054.6716	0.7	9	3	2082.3782	0.2
18	12	2019.1643	0.3	13	6	2054.7505	0.7	9	2	2082.4094	0.2
18	11	2019.2766	0.5	13	5	2054.8218	0.7	9	1	2082.4094	0.2
17	16	2025.7751	0.1	13	4	2054.8801	0.7	9	0	2082.4094	0.2
17	15	2025.8665	0.1	13	1	2054.9700	0.1	8	7	2088.9702	1.0
17	14	2025.9595	0.2	13	0	2054.9700	0.1	8	6	2089.0342	1.0
17	13	2026.0618	0.1	12	11	2061.2297	0.7	8	5	2089.0879	1.0
17	12	2026.1465	0.5	12	10	2061.3225	1.0	8	4	2089.1335	1.0
17	11	2026.2561	0.4	12	9	2061.4146	0.7	8	3	2089.1736	0.3
17	10	2026.3694	0.1	12	8	2061.5005	0.5	8	2	2089.2092	0.2
16	9	2033.6572	0.1	12	7	2061.5569	0.5	8	1	2089.2092	0.2
16	8	2033.7271	0.1	12	6	2061.6191	0.5	8	0	2089.2092	0.2
16	7	2033.8320	0.5	12	5	2061.6726	0.1	7	6	2095.8152	1.0
16	6	2033.8923	0.2	12	4	2061.7251	0.1	7	5	2095.8691	1.0
16	5	2033.9797	0.3	12	3	2061.8110	0.2	7	4	2095.9138	0.5
16	4	2034.0029	0.2	12	2	2061.8586	0.4	7	3	2095.9509	0.3
16	3	2034.0784	0.5	12	1	2061.9070	0.1	7	2	2095.9834	0.2
15	14	2040.0715	0.1	12	0	2061.9290	0.1	7	1	2095.9834	0.2
15	13	2040.1885	0.3	11	10	2068.2283	0.3	7	0	2095.9834	0.2
15	12	2040.3110	0.3	11	9	2068.3215	1.0	6	5	2102.6216	1.0
15	11	2040.4167	0.1	11	8	2068.4119	1.0	6	4	2102.6648	0.7
15	10	2040.5374	0.5	11	7	2068.4902	0.7	6	3	2102.6997	0.3
15	9	2040.6404	1.0	11	6	2068.5603	0.5	6	2	2102.7336	0.2
15	8	2040.7280	0.3	11	5	2068.6187	0.4	6	1	2102.7336	0.2
15	7	2040.7952	0.5	11	4	2068.6738	0.1	6	0	2102.7336	0.2
15	6	2040.8555	1.0	11	3	2068.7141	0.1	5	4	2109.3857	0.7
15	5	2040.9397	0.1	11	2	2068.7583	0.1	5	3	2109.4236	0.3
14	13	2047.1509	0.5	11	1	2068.7583	0.1	5	2	2109.4514	0.1
14	12	2047.2610	0.2	11	0	2068.7583	0.1	5	1	2109.4514	0.1
14	11	2047.3684	0.1	10	9	2075.1833	0.4	5	0	2109.4514	0.1
14	10	2047.4700	0.1	10	8	2075.2588	0.7	4	3	2116.1121	0.2
14	9	2047.5735	0.5	10	7	2075.3342	1.0	4	2	2116.1396	0.1
14	8	2047.6626	0.7	10	6	2075.3999	0.7	4	1	2116.1396	0.1
14	7	2047.7654	0.7	10	5	2075.4622	1.0	4	0	2116.1396	0.1
14	6	2047.8074	0.1	10	4	2075.5127	0.5	3	2	2122.7961	0.7
14	5	2047.8728	0.7	10	3	2075.5549	0.3	3	1	2122.7961	0.7
14	3	2048.0176	0.7	10	2	2075.5901	0.2	3	0	2122.7961	0.7
14	1	2048.0647	0.1	10	1	2075.5901	0.2	2	1	2129.4216	0.7
14	0	2048.0647	0.1	10	0	2075.5901	0.2	2	0	2129.4216	0.7
13	12	2054.2083	0.7	9	8	2082.0901	0.5	1	0	2136.0217	1.0
13	11	2054.3096	0.7	9	7	2082.1624	1.0				

[a] Frequencies are in cm^{-1}.

TABLE II

Observed $^{Q}Q_{K}(J)$ Transitions in ν_2 of ClD_3

J	K	Freq.[a]	Wt.	J	K	Freq.	Wt.	J	K	Freq.	Wt.
22	22	2131.6914	0.2	16	10	2136.9907	0.7	9	5	2140.8645	0.7
21	21	2132.6157	0.7	15	15	2137.3469	0.3	9	4	2140.9033	0.3
21	20	2132.6462	0.1	15	8	2137.9580	0.5	9	3	2140.9390	0.3
21	19	2132.7031	0.2	14	14	2138.0034	0.7	9	2	2140.9675	0.1
21	18	2132.7700	1.0	14	13	2138.0896	0.5	8	8	2141.0183	0.5
21	17	2132.8345	0.5	14	12	2138.1946	1.0	8	7	2141.0757	0.7
21	16	2132.8733	0.7	14	11	2138.2800	1.0	8	6	2141.1323	0.7
21	15	2132.9346	1.0	14	10	2138.3647	0.7	8	5	2141.1797	0.5
20	20	2133.4944	0.3	14	9	2138.4512	0.7	8	4	2141.2253	0.7
20	19	2133.5176	0.3	14	8	2138.5469	0.7	8	3	2141.2576	0.3
20	18	2133.5574	0.7	13	13	2138.6130	1.0	8	2	2141.2820	0.1
20	17	2133.6152	0.7	13	12	2138.6929	0.3	8	1	2141.2820	0.1
20	16	2133.6841	0.5	13	11	2138.7786	0.7	7	7	2141.3667	0.7
20	15	2133.7246	0.3	13	10	2138.8591	0.7	7	6	2141.4189	0.7
20	14	2133.8164	1.0	13	9	2138.9397	1.0	7	5	2141.4707	0.7
19	19	2134.3430	0.5	13	8	2139.0171	1.0	7	4	2141.5105	0.5
19	18	2134.3762	0.5	13	7	2139.1045	0.5	7	3	2141.5442	0.3
19	17	2134.4260	0.7	13	6	2139.1802	0.5	7	2	2141.5662	0.1
19	16	2134.4832	0.7	12	12	2139.1802	0.5	7	1	2141.5662	0.1
19	15	2134.5420	0.3	12	11	2139.2559	1.0	6	6	2141.6636	0.5
19	14	2134.6018	0.2	12	10	2139.3323	1.0	6	5	2141.7185	0.7
18	18	2135.1484	1.0	12	9	2139.4124	0.5	6	4	2141.7610	0.5
18	17	2135.1919	0.5	12	8	2139.4822	1.0	6	3	2141.7939	0.3
18	16	2135.2192	0.3	12	7	2139.5486	1.0	6	2	2141.8186	0.1
18	15	2135.2483	0.3	12	6	2139.6160	1.0	6	1	2141.8186	0.1
18	13	2135.3098	0.2	11	11	2139.6951	0.2	5	5	2141.9363	0.7
17	17	2135.9119	0.7	11	10	2139.7734	1.0	5	4	2141.9768	0.4
17	16	2135.9602	0.5	11	9	2139.8450	1.0	5	3	2142.0083	0.2
17	15	2136.0217	1.0	11	8	2139.9158	0.2	5	2	2142.0337	0.1
17	14	2136.0859	0.5	11	7	2139.9695	0.5	5	1	2142.0598	0.1
17	13	2136.1660	0.5	11	6	2140.0142	0.7	4	4	2142.1558	0.5
17	12	2136.2595	0.1	10	10	2140.1836	0.7	4	3	2142.1887	0.1
17	11	2136.3455	0.1	10	9	2140.2637	0.1	4	2	2142.2107	0.1
17	10	2136.3921	0.1	10	8	2140.3396	1.0	4	1	2142.2107	0.1
17	9	2136.4622	0.5	10	7	2140.4055	1.0	3	3	2142.3286	0.2
17	8	2136.5181	0.2	10	6	2140.4629	1.0	3	2	2142.3447	0.1
16	16	2136.6216	1.0	10	5	2140.5142	1.0	3	1	2142.3447	0.1
16	15	2136.6851	1.0	10	4	2140.5598	0.5	2	2	2142.4609	0.5
16	14	2136.7444	1.0	9	9	2140.6182	0.2	2	1	2142.4609	0.5
16	13	2136.8079	1.0	9	8	2140.6880	1.0	1	1	2142.5415	1.0
16	12	2136.8655	0.7	9	7	2140.7505	1.0				
16	11	2136.9290	0.2	9	6	2140.8113	1.0				

[a]Frequencies are in cm^{-1}.

TABLE III

Observed $^{Q}R_{K}(J)$ Transitions in ν_2 of CHD_3

J	K	Freq.[a]	Wt.	J	K	Freq.	Wt.	J	K	Freq.	Wt.
0	0	2149.1094	1.0	7	5	2193.5576	0.5	10	5	2211.9905	0.2
1	1	2155.5896	1.0	7	4	2193.5959	0.4	10	4	2212.0764	0.2
1	0	2155.5896	1.0	7	3	2193.6313	0.2	10	3	2212.1104	0.2
2	2	2162.0374	1.0	7	2	2193.6497	0.1	10	2	2212.1584	0.1
2	1	2162.0374	1.0	7	1	2193.6497	0.1	10	1	2212.1584	0.1
2	0	2162.0374	1.0	7	0	2193.6497	0.1	10	0	2212.1584	0.1
3	3	2168.4214	0.5	8	8	2199.6033	0.2	11	11	2217.7275	0.7
3	2	2168.4468	0.5	8	7	2199.6597	0.7	11	10	2217.7942	0.7
3	1	2168.4468	0.5	8	6	2199.7112	0.7	11	9	2217.8447	0.7
3	0	2168.4468	0.5	8	5	2199.7559	0.5	11	8	2217.8994	0.2
4	4	2174.7561	0.3	8	4	2199.7939	0.3	11	7	2217.9539	1.0
4	3	2174.7947	0.2	8	3	2199.8455	0.1	11	6	2218.0076	1.0
4	2	2174.7947	0.2	8	2	2199.8455	0.1	11	5	2218.0613	0.7
4	1	2174.7947	0.2	8	1	2199.8455	0.1	11	4	2218.1006	0.7
4	0	2174.7947	0.2	8	0	2199.8455	0.1	12	12	2223.6614	0.5
5	5	2181.0471	0.3	9	9	2205.7061	1.0	12	11	2223.7207	0.5
5	4	2181.0835	0.2	9	8	2205.7732	0.7	12	10	2223.7729	1.0
5	3	2181.1135	0.1	9	7	2205.8284	0.7	12	9	2223.8396	1.0
5	2	2181.1331	0.1	9	6	2205.8767	0.7	12	8	2223.9050	1.0
5	1	2181.1331	0.1	9	5	2205.9202	0.5	12	7	2223.9736	1.0
5	0	2181.1331	0.1	9	4	2205.9604	0.2	12	6	2224.0281	0.3
6	6	2187.2803	0.7	9	3	2205.9961	0.1	12	5	2224.0576	0.3
6	5	2187.3230	0.7	9	2	2205.9961	0.1	13	13	2229.5479	0.7
6	4	2187.3674	0.2	9	1	2205.9961	0.1	13	12	2229.6235	0.5
6	3	2187.3960	0.1	9	0	2205.9961	0.1	13	11	2229.6721	0.5
6	2	2187.4128	0.1	10	10	2211.7310	0.2	13	10	2229.7593	0.5
6	1	2187.4128	0.1	10	9	2211.7917	0.5	13	9	2229.8069	0.3
6	0	2187.4128	0.1	10	8	2211.8379	0.5	13	8	2229.8682	0.2
7	7	2193.4692	0.7	10	7	2211.8906	0.3	13	7	2229.8931	0.2
7	6	2193.5154	0.5	10	6	2211.9236	0.3	13	5	2229.9915	0.5

[a] Frequencies are in cm^{-1}.

TABLE IV

GROUND STATE PARAMETERS FOR CHD_3[a]

B_o	$3.279053 \pm 0.000061\ cm^{-1}$
D_o^J	$5.010 \times 10^{-5} \pm 0.019 \times 10^{-5}\ cm^{-1}$
D_o^{JK}	$-4.030 \times 10^{-5} \pm 0.069 \times 10^{-5}\ cm^{-1}$
H_o^J	$1.020 \times 10^{-8} \pm 0.059 \times 10^{-8}\ cm^{-1}$
H_o^{JK}	$-3.80 \times 10^{-8} \pm 0.15 \times 10^{-8}\ cm^{-1}$
H_o^{KJ}	$5.15 \times 10^{-8} \pm 0.40 \times 10^{-8}\ cm^{-1}$

[a]Error limits given correspond to a 95 percent confidence interval (8).

TABLE V

RESULTS OF PREVIOUS STUDIES

Band	$B_o(cm^{-1})$	$D_o^{JK}(cm^{-1})$	$D_o^J(cm^{-1})$
$\nu_1+\nu_2$ [a]	3.2795 ± 0.0005	$(-4.0 \pm 1.2) \times 10^{-5}$	$(5.2 \pm 0.5) \times 10^{-5}$
$2\nu_5$ [b]	3.278 ± 0.001	4×10^{-5}	
ν_1 [c]	3.2792		4.6×10^{-5}
$2\nu_1$ [d]	3.2777	-4×10^{-5}	3.9×10^{-5}
$4\nu_1$ [e]	3.2787 ± 0.001	-3.5×10^{-5}	4.6×10^{-5}
$3\nu_1$ [e]	3.2784		5×10^{-5}

[a] Blass and Edwards (3).

[b] Allen and Plyler (9).

[c] Rea and Thompson (2).

[d] Wiggins, Shull, Bennett, and Rank (10).

[e] Bovey (11).

TABLE VI

MOLECULAR PARAMETERS FOR ν_2[a]

ν_o	2142.5776
α_2^B	$1.7549 \times 10^{-2} \pm 0.0019 \times 10^{-2}$
$\alpha_2^A - \alpha_2^B$	$4.700 \times 10^{-3} \pm 0.022 \times 10^{-3}$
β_2^K	$1.0045 \times 10^{-5} \pm 0.0064 \times 10^{-5}$
β_2^{JK}	$-7.576 \times 10^{-6} \pm 0.054 \times 10^{-6}$
β_2^J	$-9.03 \times 10^{-7} \pm 0.43 \times 10^{-7}$

[a]Error limits given correspond to a 95 percent confidence interval (8).

List of Symbols

ν	low case Greek letter 'nu'
α	lower case Greek letter 'alpha'
β	lower case Greek Letter 'beta'
$>$	'greater than' sign
$<$	'less than' sign
Δ	upper case Greek letter 'delta'
$\propto$	'proportional to' sign
$\sqrt{}$	square root symbol