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A Table of Rotational Constants of Symmetric Top Molecules Giving Rise to Microwave Spectra*

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This paper lists, in order of increasing value, the "B" rotational constants of most of the linear and symmetric top molecules which have been observed by microwave spectroscopy. Also are listed the microwave spectral lines which have been observed for the asymmetric tops water and formaldehyde. These data are useful for making a quick selection of a molecule which has a spectral line close to some previously selected frequency.

Key words: Asymmetric, linear, and symmetric top molecules; "B" rotational constants; formaldehyde; microwave spectra; spectral lines; water.

Nowadays there are a number of actual and potential situations in which one would like to select a molecule to have a spectral line close to some previously specified frequency. For one thing, the transitions of light linear or symmetric top molecules, which lie in almost but not exact harmonic relationship, are used to tune up millimeter wave spectrographs. For another, there is a great interest in devising experiments, many involving lasers, in which a spectral line, or one of the harmonics of its frequency, nearly coincides with a spectral line of another substance. In addition there might be practical applications, such as in a communications system, in which it may be desired to build a molecular frequency standard with its fundamental close to some previously chosen frequency.

As an aid to making such a selection, herewith in table 1 is presented, in order of increasing value, the "B" rotational constants of most of the linear and symmetric top molecules which are listed in "Microwave Spectral Tables," National Bureau of Standards, Monograph 70.[1] From the simple well-known formula given in eq (1) it is possible to get a very good approximation of the frequencies of nearly all of the rotational lines of these molecules. The frequency

$$f = 2BJ, \tag{1}$$

where J is any integer, which is the quantum number giving the total angular momentum (not including nuclear spin) of the upper state giving rise to the transition. In table 1, values of B are given for only one isotopic species of each molecule, generally the most abundant one. The values for other isotopic species may be easily determined from the fact that B is inversely proportional to the reduced mass of the molecule. Also listed in table 1 are the common names of the molecules to aid in referring to handbooks giving physical properties and to the catalogs of chemical companies.

The values of B given in table 1 were obtained from the same punched computer cards which served as the basis of the "Microwave Spectral Tables." A program was written for selecting the values in accordance with the present philosophy, arranging the values in ascend-

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[1] These Tables may be obtained through the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.
The following volumes have been published:
Volume I: Diatomic Molecules, by P. F. Wacker, M. Mizushima, J. D. Petersen, and J. R. Ballard, December 15, 1964.
Volume II: Line Strengths of Asymmetric Rotors, by P. F. Wacker and M. R. Pratto, December 15, 1964.
Volume IV: Polyatomic Molecules Without Internal Rotation, M. S. Cord, J. D. Petersen, M. S. Lojko, and R. H. Haas, October 1968.
Volume V: Spectral Line Listing, by M. S. Cord, M. S. Lojko, and J. D. Petersen, June 1968.
Publication of the remaining volume is expected shortly:
Volume III: Polyatomic Molecules With Internal Rotation, P. F. Wacker, M. S. Cord, D. G. Burkhard, J. D. Petersen, and R. F. Kukol.

ing order, and printing out the result. In this tabulation, it has not been practical to distinguish between ground vibrational state (B_o) and equilibrium state (B_e) values. In most cases, however, for polyatomic molecules the values given pertain to the ground vibrational state while for diatomic molecules they pertain to the equilibrium state. However, the difference between values of these quantities for the same molecule is probably smaller than the errors associated with eq (1) which result from the neglect of such effects as centrifugal distortion and hyperfine effects.

Accordingly, it is appropriate to give some general discussion of the tables. The present series of volumes are based upon a thorough search of the literature of microwave spectroscopy. The cut-off date of the search differs slightly from volume to volume but is approximately 1961 for all of them. In addition, through the cooperation of numerous investigators, much unpublished data and data published in sources not widely available have been included. In a number of cases where important data after the official cut-off date happened to be conveniently available, they were included, but inclusion of post-cut-off data was determined by convenience and nothing else. A critical selection was made, and the selected data on frequencies and molecular constants were transcribed upon punched cards. The cards were checked against the original sources. Except for a few nonstandard situations, all final print-out was made direct from the cards by use of suitable programs. The present series of volumes were carried out in accordance with a plan developed by Paul W. Wacker. It received sponsorship of the Office of Standard Reference Data of the National Bureau of Standards when it became established. It is likely that in due time supplements to the present series will be published under sponsorship of the Office.

Volume V, which lists the measured frequencies of spectral lines in order of frequency, is also useful in giving direct answers to questions of the type described in the opening paragraph above. Indeed most of the time it may be more useful than table 1 and eq (1). However, the present material is useful in providing some answers not contained in Volume V, and therefore availability of the present material is highly desirable. One reason is that Volume V contains only lines that have actually been observed and measured accurately. However, there exist many lines which are observable but which have not been observed, and there are others which have been observed but not measured accurately and not published. In addition, Volume V contains very few entries above 300 GHz and none above 500 GHz. At the same time, the development of submillimeter lasers has stimulated a great interest in the frequencies of spectral lines up to a few thousand megahertz. The material given here can be used to give good approximations of the frequencies of many spectral lines which are involved in either of these two categories. Once eq (1) has been used to select a molecular transition, the frequency may be computed more exactly by including such effects as centrifugal distortion and hyperfine interactions by methods contained in textbooks but beyond the scope of this paper.

TABLE 1. *"B" Rotational constants of symmetric top and linear molecules*

B(MHz)	Molecule name	Isotopic species [a]
708.3579	Cesium Iodide	$Cs^{133}I^{127}$
725.9	1-Bromo-Bicyclo(2,2,2)Octane	$C_8^{12}H_{13}Br^{79}$
729.8	Benzene Chromium Tricarbonyl	$C_6^{12}H_6Cr^{52}(C^{12}O^{16})_3$
788.0	Methyl Mercuric Iodide	$C^{12}H_3H_g{}^bI^b$
817.510	Thallium Iodide	$TI^{205}I^{127}$
891.69	1-Chloro-3,3-Dimethyl-1-Butyne	$(C^{12}H_3)_3C^{12}C^{12}\equiv C^{12}Cl^{35}$
984.3166	Rubidium Iodide	$Rb^{85}I^{127}$
996.4	Phosphorus Tribromide	$P^bBr_3^{79}$
1081.343	Cesium Bromide	$Cs^{133}Br^{79}$
1096.42	Trimethyliodosilane	$(C^{12}H_3)_3Si^{28}I^{127}$
1104.95	Indium Iodide	$In^{115}I^{127}$
1142.86	Methyl Mercuric Bromide	$C^{12}H_3Hg^{198}Br^{79}$
1247.61	Tribromomethane	$C^{12}HBr_3^{79}$
1259.02	1-Iodopropyne	$H_3C^{12}C^{12}\equiv C^{12}I^{127}$
1259.25	Nickel Cyclopentadienyl Nitrosyl	$C_5^{12}H_5N^{14}Ni^{58}O^{16}$
1297.409	Thallium Bromide	$TI^{205}Br^{79}$
1369.70	1,1,1-Trifluoro-2-Butyne	$C^{12}H_3C^{12}\equiv C^{12}C^{12}F_3^{19}$
1402.64	Thiophosphoryl Chloride	$S^{32}P^{31}Cl_3^{35}$
1424.840	Rubidium Bromide	$Rb^{85}Br^{79}$
1461.95	Trimethylbromosilane	$(C^{12}H_3)_3Si^{28}Br^{79}$
1467.98	Cyclopentadienyl Thallium	$C_5^{12}H_5TI^{203}$
1497.	Bismuth Trichloride	$Bi^{209}Cl_3^{35}$
1516.018	Silyl Isothiocyanate	$Si^{28}H_3N^{14}C^{12}S^{32}$
1523.23	Trifluoroiodomethane	$C^{12}F_3^{19}I^{127}$
1549.98	Bromotrifluorosilane	$Si^{28}F_3^{19}Br^{79}$
1561.11	1-Bromopropyne	$H_3C^{12}C^{12}\equiv C^{12}Br^{79}$

[a] The superscript b means that the particular isotope was not specified.

TABLE 1. *"B" Rotational constants of symmetric top and linear molecules*—Continued

B(MHz)	Molecule name	Isotopic species [a]
1562.	2-Iodo-2-Methylpropane	$(C^{12}H_3)_3C^{12}I^{127}$
1573.7	Trimethylamine-Trimethylborane	$(C^{12}H_3)_3N^{14} \cdot B^{11}(C^{12}H_3)_3$
1584.122	Thiocarbonyl Telluride	$S^{32}C^{12}Te^{122}$
1599.3	Methyltrichlorogermane	$C^{12}H_3Ge^{b}Cl^{35}_3$
1667.2	Trichloroacetonitrile	$C^{12}Cl^{35}_3C^{12}N^{14}$
1670.14	Indium Bromide	$In^{115}Br^{79}$
1706.86	Gallium Monoiodide	$Ga^{69}I^{127}$
1750.	Trifluoroborane-trimethylamine	$F^{19}_3B^{b} \cdot N^{b}(C^{12}H_3)_3$
1753.9	Antimony Trichloride	$Sb^{121}Cl^{35}_3$
1769.836	Methyltrichlorosilane	$C^{12}H_3Si^{28}Cl^{35}_3$
1825.012	Potassium Iodide	$K^{39}I^{127}$
2001.56	Thiocarbonyl Selenide	$S^{32}C^{12}Se^{82}$
2015.20	Phosphoryl Chloride	$P^{31}O^{16}Cl^{35}_3$
2035.741	Penta-1,3-Diyne	$H_3C^{12}C^{12}\equiv C^{12}C^{12}\equiv C^{12}H$
2044.2	2-Bromo-2-Methylpropane	$(C^{12}H_3)_3C^{12}Br^{79}$
2065.73	2-Butynenitrile	$H_3C^{12}C^{12}\equiv C^{12}C^{12}N^{14}$
2077.48	Methyl Mercuric Chloride	$C^{12}H_3Hg^{198}Cl^{35}$
2094.20	Rhenium Trioxychloride	$Re^{185}O^{16}_3Cl^{35}$
2098.06	Bromotrifluoromethane	$C^{12}F^{19}_3Br^{79}$
2147.2	Arsenic Trichloride	$As^{75}Cl^{35}_3$
2161.208	Cesium Chloride	$Cs^{133}Cl^{35}$
2168.52	Chlorotrifluorogermane	$Ge^{70}F^{19}_3Cl^{35}$
2172.75	Trichlorogermane	$Ge^{70}HCl^{35}_3$
2197.441	Trimethylchlorosilane	$(C^{12}H_3)_3Si^{28}Cl^{35}$
2232.271	1-Chloropropyne	$C^{12}H_3C^{12}\equiv C^{12}Cl^{35}$
2326.	Phosphorus Tricyanide	$P^{b}(C^{12}N^{14})_3$
2372.6	1,1,1-Trichloroethane	$C^{12}H_3C^{12}Cl^{35}_3$
2431.4	Quinuclidine	$C^{12}_7H_{13}N^{14}$
2434.953	Potassium Bromide	$K^{39}Br^{79}$
2438.57	Bromogermane	$Ge^{70}H_3Br^{79}$
2465.39	Trichlorofluoromethane	$C^{12}Cl^{35}_3F^{19}$
2472.489	Trichlorosilane	$Si^{28}HCl^{35}_3$
2477.79	Chlorotrifluorosilane	$Si^{28}F^{19}_3Cl^{35}$
2481.99	Gallium Monobromide	$Ga^{69}Br^{79}$
2617.1	Phosphorus Trichloride	$P^{31}Cl^{35}_3$
2657.63	Thiophosphoryl Fluoride	$S^{32}P^{31}F^{19}_3$
2683.18	1,1-Dimethyl-3-Butyne	$(C^{12}H_3)_3C^{12}C^{12}\equiv C^{12}H$
2743.913	Thallium Chloride	$Tl^{203}Cl^{35}$
2749.89	2,2-Dimethylpropanenitrile	$(C^{12}H_3)_3C^{12}C^{12}N^{14}$
2767.414	Rubidium Chloride	$Rb^{85}Cl^{35}$
2877.93	3,3,3-Trifluoro-1-Propyne	$C^{12}F^{19}_3C^{12}=C^{12}H$
2945.528	Trifluoroacetonitrile	$C^{12}F^{19}_3C^{12}N^{14}$
3017.69	2-Chloro-2-Methylpropane	$(C^{12}H_3)_3C^{12}Cl^{35}$
3215.52	Iodosilane	$Si^{28}H_3I^{127}$
3225.578	Cyanogen Iodide	$I^{127}C^{12}N^{14}$
3257.	Methyltrifluorogermane	$C^{12}H_3Ge^{b}F^{19}_3$
3269.47	Indium Chloride	$In^{115}Cl^{35}$
3301.94	Trichloromethane	$C^{12}HCl^{35}_3$
3335.56	Chlorotrifluoromethane	$C^{12}F^{19}_3Cl^{35}$
3411.00	Trimethylfluorosilane	$(C^{12}H_3)_3Si^{28}F^{19}$
3422.300	Iodine Monochloride	$I^{127}Cl^{35}$
3531.778	Sodium Iodide	$Na^{23}I^{127}$
3566.801	Rhenium Trioxyfluoride	$Re^{185}O^{16}_3F^{19}$
3715.66	Methyltrifluorosilane	$C^{12}H_3Si^{28}F^{19}_3$
3856.399	Potassium Chloride	$K^{39}Cl^{35}$
4095.786	Carbonyl Selenide	$O^{16}C^{12}Se^{74}$
4120.230	Cyanogen Bromide	$Br^{79}C^{12}N^{14}$
4129.106	Manganese Trioxyfluoride	$Mn^{55}O^{16}_3F^{19}$
4321.72	Bromosilane	$Si^{28}H_3Br^{79}$
4401.71	Chlorogermane	$Ge^{70}H_3Cl^{35}$
4493.73	Gallium Monochloride	$Ga^{69}Cl^{35}$
4534.52	Sodium Bromide	$Na^{23}Br^{79}$
4549.07	Propiolonitrile	$HC^{12}\equiv C^{12}C^{12}N^{14}$
4570.92	Bromine Monochloride	$Br^{79}Cl^{35}$
4594.262	Phosphoryl Fluoride	$P^{31}O^{16}F^{19}_3$
4636.24	Trifluorosulfur Nitride	$N^{14}S^{32}F^{19}_3$

[a] The superscript b means that the particular isotope was not specified.

TABLE 1. *"B" Rotational constants of symmetric top and linear molecules*—Continued

B(MHz)	Molecule name	Isotopic species [a]
4712.15	2-Fluoro-2-Methylpropane	$(C^{12}H_3)_3C^{12}F^{19}$
4724.98	Trimethylarsine	$(C^{12}H_3)_3As^{75}$
4972.7	Silyl Cyanide	$H_3Si^{28}C^{12}N^{14}$
5185.14	1,1,1-Trifluoroethane	$C^{12}H_3C^{12}F_3^{19}$
5260.66	Perchlorylfluoride	$Cl^{35}O_3^{16}F^{19}$
5273.6	1,3,5-Trioxane	$O^{16}*C^{12}H_2O^{16}C^{12}H_2O^{16}C^{12}*H_2$
5345.15	Trimethylsilane	$(C^{12}H_3)_3Si^{28}H$
5527.34	Cesium Fluoride	$Cs^{13}F^{19}$
5684.24	Chloroacetylene	$HC^{12}\equiv C^{12}Cl^{35}$
5816.24	Trimethylphosphine	$(C^{12}H_3)_3P^{31}$
5878.971	Arsenic Trifluoride	$As^{75}F_3^{19}$
5970.831	Cyanogen Chloride	$Cl^{35}C^{12}N^{14}$
6081.480	Carbonyl Sulfide	$O^{16}C^{12}S^{32}$
6537.07	Sodium Chloride	$Na^{23}Cl^{35}$
6673.8	Chlorosilane	$Si^{28}H_3Cl^{35}$
6695.46	Thallium Fluoride	$TI^{203}F^{19}$
6906.35	Methyltin	$C^{12}H_3Sn^{118}H_3$
7208.049	Trifluorosilane	$Si^{28}F_3^{19}H$
7501.30	Iodomethane	$C^{12}H_3I^{127}$
7789.45	2-Methylpropane	$(C^{12}H_3)_3C^{12}H$
7819.900	Phosphorus Trifluoride	$P^{31}F_3^{19}$
8545.84	Propyne	$C^{12}H_3C^{12}\equiv C^{12}H$
8710.65	Methylgermane	$C^{12}H_3Ge^{70}H_3$
8720.86	Trimethylamine	$(C^{12}H_3)_3N^{14}$
8979.94	Carbonyl Borane	$H_3B^{10}C^{12}O^{16}$
9198.83	Acetonitrile	$C^{12}H_3C^{12}N^{14}$
9568.20	Bromomethane	$C^{12}H_3Br^{79}$
9706.22	Fluoroacetylene	$HC^{12}\equiv C^{12}F^{19}$
10052.88	Methyl Isocyanide	$C^{12}H_3N^{14}C^{12}$
10348.74	Trifluoromethane	$C^{12}HF_3^{19}$
10554.20	Cyanogen Fluoride	$F^{19}C^{12}N^{14}$
10680.96	Nitrogen Trifluoride	$N^{14}F_3^{19}$
10706.9	Bromine Monofluoride	$Br^{79}F^{19}$
10968.96	Methylsilane	$C^{12}H_3Si^{28}H_3$
12561.64	Nitrous Oxide	$N_2^{14}O^{16}$
13292.84	Chloromethane	$C^{12}H_3Cl^{35}$
14327.9	Fluorosilane	$Si^{28}H_3F^{19}$
15381.99	Lithium Iodide	Li^6I^{127}
15483.69	Fluorine Chloride	$F^{19}Cl^{35}$
19162.32	Lithium Bromide	Li^6Br^{81}
24584.35	Carbon Monosulfide	$C^{12}S^{32}$
25530.59	Fluoromethane	$C^{12}H_3F^{19}$
43100.5	Oxygen	O_2^{16}
44315.99	Hydrocyanic Acid	$HC^{12}N^{14}$
51109.51	Nitric Oxide	$N^{14}O^{16}$
57898.568	Carbon Monoxide	$C^{12}O^{16}$
88031.92	Stibine	$Sb^{121}H_3$
112468.5	Arsine	$As^{75}H_3$
128600	Hydrogen Bromide	DBr^{79}
133478.3	Phosphine	$P^{31}H_3$
163340.1	Hydrogen Chloride	DCl^{35}
195229.1	Hydrogen Iodide	HI^{127}
298000	Ammonia	$N^{14}H_3$

[a] The superscript b means that the particular isotope was not specified.

Of course, there are molecular transitions other than the rotational ones of symmetric top molecules that can serve the purposes alluded to in the introductory paragraph. The well known inversion spectrum of ammonia has been used for this purpose. The frequencies of the lines are tabulated in Volume V and elsewhere. The lines of asymmetric tops may be used too, if they are listed in Volume V or known by some other means. However, the calculation of their frequencies from molecular data cannot be done in closed form, and even rough estimates can sometimes be very laborious. Two of these molecules, water and formaldehyde, deserve special mention because samples are easy to obtain, and the lines from them are very strong and distributed widely over the spectrum. For convenience, the listings of spectral lines of these molecules, contained in Volume IV of NBS Monograph 70, are reprinted here in tables 2 and 3 respectively.

TABLE 2. *Microwave spectral lines of water*

The Rotational Quantum Numbers are, respectively, J, K_{-1}, *and* K_{+1} upper state followed by J, K_{-1}, and K_{+1} of the lower state.

All transitions pertain to ground vibrational state.

Isotopic species	Rotational quantum Nos.	Hyperfine				Frequency MHz	Acc. ±MHz
		F_1'	F'	F_1	F		
H_3O^{16}	3, 1, 3 ← 2, 2, 0					183 311.30	.30
	6, 1, 6 ← 5, 2, 3					22 235.22	.05
HDO^{16}	1, 1, 0 ← 1, 1, 1					80 578.15	
	2, 1, 1 ← 2, 1, 2					241 561.3	
	2, 2, 1 ← 2, 2, 0	1	3/2	2	5/2	10 278.0796	.001
	2, 2, 1 ← 2, 2, 0	3	5/2	3	7/2	10 278.1365	.001
	2, 2, 1 ← 2, 2, 0	1	1/2	1	3/2	10 278.1681	.001
	2, 2, 1 ← 2, 2, 0	3	5/2	1	3/2	10 278.2255	.001
	2, 2, 1 ← 2, 2, 0					10 278.2455	.001
	2, 2, 1 ← 2, 2, 0	1	3/2	3	5/2	10 278.2643	.001
	2, 2, 1 ← 2, 2, 0	1	3/2	1	1/2	10 278.3234	.001
	2, 2, 1 ← 2, 2, 0	3	7/2	3	5/2	10 278.3554	.001
	2, 2, 1 ← 2, 2, 0	2	5/2	1	3/2	10 278.4126	.001
	3, 2, 1 ← 3, 2, 2					50 236.30	
	3, 3, 0 ← 3, 3, 1	3	5/2	2	3/2	824.4754	.002
	3, 3, 0 ← 3, 3, 1	4	9/2	4	7/2	824.5074	.002
	3, 3, 0 ← 3, 3, 1	3	5/2	4	7/2	824.5247	.002
	3, 3, 0 ← 3, 3, 1	3	7/2	3	5/2	824.5488	.002
	3, 3, 0 ← 3, 3, 1	3	7/2	4	9/2	824.5685	.002
	3, 3, 0 ← 3, 3, 1	2	5/2	4	7/2	824.6042	.002
	3, 3, 0 ← 3, 3, 1					824.6706	.002
	3, 3, 0 ← 3, 3, 1	2	5/2	4	7/2	824.7419	.002
	3, 3, 0 ← 3, 3, 1	3	7/2	4	9/2	824.7730	.002
	3, 3, 0 ← 3, 3, 1	3	7/2	3	5/2	824.7904	.002
	3, 3, 0 ← 3, 3, 1	3	5/2	4	7/2	824.8136	.002
	3, 3, 0 ← 3, 3, 1	4	9/2	4	7/2	824.8341	.002
	3, 3, 0 ← 3, 3, 1	3	5/2	2	3/2	824.8637	.002
	3, 2, 1 ← 4, 1, 4					20 460.40	
	4, 2, 2 ← 4, 2, 3					143 727.2	
	4, 3, 1 ← 4, 3, 2					5 702.78	
	5, 0, 5 ← 4, 2, 2					2 887.4	.1
	5, 1, 5 ← 4, 2, 2					120 778.2	
	5, 3, 2 ← 5, 3, 3					22 307.67	.05
	5, 4, 1 ← 5, 4, 2	5	11/2	5	9/2	486.266	.002
	5, 4, 1 ← 5, 4, 2	5	11/2	4	9/2	486.450	.002
	5, 4, 1 ← 5, 4, 2	5	11/2	6	13/2	486.487	.002
	5, 4, 1 ← 5, 4, 2					486.528	.002
	5, 4, 1 ← 5, 4, 2	5	11/2	6	13/2	486.569	.002
	5, 4, 1 ← 5, 4, 2	5	11/2	4	9/2	486.606	.002
	6, 1, 6 ← 5, 2, 3					138 530.4	
	6, 4, 2 ← 6, 4, 3					2 394.56	.05
	7, 1, 7 ← 6, 2, 4					26 880.38	.05
	7, 4, 3 ← 7, 4, 4					8 577.7	.1
	8, 4, 4 ← 8, 4, 5					24 884.77	.05
	9, 5, 4 ← 9, 5, 5					3 044.71	.10
	10, 5, 5 ← 10, 5, 6					8 836.95	.1
	11, 5, 6 ← 11, 5, 7					22 581.1	.2
	12, 6, 6 ← 12, 6, 7					2 961.	1.
D_2O^{16}	3, 1, 3 ← 2, 2, 0	7/2	3	5/2	2	10 919.301	.001
	3, 1, 3 ← 2, 2, 0	9/2	5	7/2	4	10 919.357	.001
	3, 1, 3 ← 2, 2, 0	5/2	4	3/2	3	10 919.521	.001
	3, 1, 3 ← 2, 2, 0	9/2	3	7/2	2	10 919.603	.001
	4, 2, 3 ← 3, 3, 0					43 414.57	

TABLE 2. *Microwave spectral lines of water*—Continued

Isotopic species	Rotational quantum Nos.	Hyperfine				Frequency MHz	Acc. ±MHz
		F_1'	F'	F_1	F		
—Continued	4, 4, 0 ← 5, 3, 3					55 482.32	
	4, 4, 1 ← 5, 3, 2					10 947.13	.05
	6, 1, 6 ← 5, 2, 3					90 916.8	
HDO^{17}	2, 2, 0 ← 2, 2, 1					10 374.56	
	3, , ← 2, ,					23 374.4	.05
	3, , ← 2, ,					23 481.6	.05
	3, , ← 2, ,					23 585.6	.05
	3, , ← 2, ,					23 646.3	.05
	3, , ← 2, ,					24 256.0	.05
	3, , ← 2, ,					24 280.5	.05
	3, , ← 2, ,					24 384.9	.5
	3, , ← 2, ,					24 472.6	.5
	3, , ← 2, ,					24 528.8	.5

TABLE 3. *Microwave spectral lines of formaldehyde*

The Rotational Quantum Numbers are, respectively, J, K_{-1}, and K_{+1} upper state followed by J, K_{-1}, and K_{+1} of the lower state.

All transitions pertain to ground vibrational state.

Isotopic species	Rotational quantum Nos.	Hyperfine				Frequency MHz	Acc. ±MHz
		F_1'	F'	F_1	F		
HC^{12}HO^{16}	1, 0, 1 ← 0, 0, 0					72 838.14	
	1, 1, 0 ← 1, 1, 1					4 829.73	.01
	2, 0, 2 ← 1, 0, 1					145 603.1	.73
	2, 1, 1 ← 1, 1, 0					150 498.2	.75
	2, 1, 2 ← 1, 1, 1					140 839.3	.70
	2, 1, 1 ← 2, 1, 2					14 488.65	
	3, 0, 3 ← 2, 0, 2					218 221.6	1.1
	3, 1, 2 ← 2, 1, 1					225 698.2	1.1
	3, 1, 3 ← 2, 1, 2					211 210.6	1.1
	3, 2, 0 ← 2, 2, 0					218 759.4	1.1
	3, 2, 2 ← 2, 2, 1					218 475.1	1.1
	3, 1, 2 ← 3, 1, 3					28 974.85	
	3, 2, 1 ← 3, 2, 2					355.586	.005
	4, 1, 3 ← 4, 1, 4					48 284.60	
	4, 2, 2 ← 4, 2, 3					1 065.85	.02
	5, 1, 4 ← 5, 1, 5					72 409.35	
	6, 2, 4 ← 6, 2, 5					4 954.76	.01
	7, 2, 5 ← 7, 2, 6					8 884.87	
	8, 2, 6 ← 8, 2, 7					14 726.74	
	8, 3, 5 ← 8, 3, 6					301.10	.01
	9, 2, 7 ← 9, 2, 8					22 965.71	
	9, 3, 6 ← 9, 3, 7					601.07	.005
	11, 2, 9 ← 11, 2,10					48 612.70	.1
	12, 3, 9 ← 12, 3,10					3 225.58	.01
	13, 3,10 ← 13, 3,11					5 136.58	.01
	14, 3,11 ← 14, 3,12					7 892.03	
	15, 3,12 ← 15, 3,13					11 753.13	
	16, 3,13 ← 16, 3,14					17 027.60	
	17, 3,14 ← 17, 3,15					24 068.31	
	19, 3,16 ← 19, 3,17					45 063.10	.1

TABLE 3. *Microwave spectral lines of formaldehyde* — Continued

Isotopic species	Rotational quantum Nos.	Hyperfine				Frequency MHz	Acc. ± MHz
		F_1'	F'	F_1	F		
$HC^{12}HO^{16}$ – Con.	20, 4,16 ← 20, 4,17					3 518.85	.5
	21, 4,17 ← 21, 4,18					5 138.57	.5
	22, 4,18 ← 22, 4,19					7 362.60	
	23, 4,19 ← 23, 4,20					10 366.51	
	24, 4,20 ← 24, 4,21					14 361.54	
	25, 4,21 ← 25, 4,22					19 595.23	
	26, 4,22 ← 26, 4,23					26 358.82	
	28, 4,24 ← 28, 4,25					45 835.58	
	31, 5,26 ← 31, 5,27					7 833.20	
	1, 1, 0 ← 1, 1, 1					4 593.26	.5
	2, 1, 1 ← 2, 1, 2					13 778.86	
	3, 1, 2 ← 3, 1, 3					27 555.73	
	4, 1, 3 ← 4, 1, 4					45 920.08	
	7, 2, 5 ← 7, 2, 6					8 012.56	.5
	9, 2, 7 ← 9, 2, 8					20 736.30	
	14, 3,11 ← 14, 3,12					6 752.31	.5
	16, 3,13 ← 16, 3,14					14 592.44	
	17, 3,14 ← 17, 3,15					20 649.30	
	18, 3,15 ← 18, 3,16					28 582.40	
$HC^{12}HO^{18}$	1, 1, 0 ← 1, 1, 1					4 388.85	.5
$DC^{12}DO^{16}$	1, 1, 0 ← 1, 1, 1					6 096.10	.02
	2, 1, 1 ← 2, 1, 2					18 287.90	
	4, 2, 2 ← 4, 2, 3					3 687.28	.04
	5, 2, 3 ← 5, 2, 4					8 519.10	
	6, 2, 4 ← 6, 2, 5					16 759.64	
	8, 3, 5 ← 8, 3, 6					2 850.62	.03
	9, 3, 6 ← 9, 3, 7					5 636.98	
	10, 3, 7 ← 10, 3, 8					10 304.64	
	13, 4, 9 ← 13, 4,10					3 079.48	.03
	14, 4,10 ← 14, 4,11					5 461.54	
	15, 4,11 ← 15, 4,12					9 259.88	
	16, 4,12 ← 16, 4,13					15 080.34	
	19, 5,14 ← 19, 5,15					4 508.39	.04
$HC^{12}DO^{16}$	1, 1, 0 ← 1, 1, 1					5 346.64	.03
	2, 1, 1 ← 2, 1, 2					16 038.06	
	3, 2, 1 ← 3, 2, 2					644.893	.005
	5, 2, 3 ← 5, 2, 4					4 489.08	.03
	6, 2, 4 ← 6, 2, 5					8 922.59	
	7, 2, 5 ← 7, 2, 6					15 907.38	
	10, 3, 7 ← 10, 3, 8					3 283.09	.03
	11, 3, 8 ← 11, 3, 9					5 702.6	
	12, 3, 9 ← 12, 3,10					9 412.51	
	13, 3,10 ← 13, 3,11					14 873.02	
	16, 4,12 ← 16, 4,13					2 946.67	.03
	17, 4,13 ← 17, 4,14					4 713.90	
	18, 4,14 ← 18, 4,15					7 322.35	
	19, 4,15 ← 19, 4,16					11 074.30	
	23, 5,18 ← 23, 5,19					3 330.66	.04
	24, 5,19 ← 24, 5,20					5 018.25	
$HC^{12}DO^{16}$	1, 1, 0 ← 1, 1, 1					5 156.19	.10

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