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TABLE OF VIBRATIONAL FORCE CONSTANTS*

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Contents

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Introduction

The potential energy of a diatomic molecule may be expanded as

$$2U(r) = F_2(r-r_e)^2 + F_3(r-r_e)^3 + F_4(r-r_e)^4 + \cdots \quad (1)$$

where F_2, F_3, F_4, $\cdots$ are the quadratic, cubic, quartic, $\cdots$ force constants and r_e is the equilibrium internuclear distance. Another form is

$$2U(r) = 2a_0\xi^2(1 + a_1\xi + a_2\xi^2 + \cdots) \quad (2)$$

where

$$\xi = (r-r_e)/r_e \quad (3)$$

$$a_0 = \tfrac{1}{2} F_2 r_e^{\,2} \quad (4)$$

and

$$a_n = F_n r_e^{\,n}/F_2 \quad (5)$$

Several texts[1-3] discuss in detail the calculation of force constants from spectroscopic data. The analysis of vibration-rotation bands of diatomic molecules is usually based on an expansion of the energy levels:

$$G(V) = \omega_e V - \omega_e x_e V^2 + \omega_e y_e V^3 + \omega_e z_e V^4 + \cdots \quad (6)$$

$$F(J) = B_v P^2 - D_e P^4 + H_e P^6 + \cdots \quad (7)$$

where

$$B_v = B_e - \alpha_e V + \gamma_e V^2 + \cdots \quad (8)$$

and

$$V = (v + \tfrac{1}{2}),\ P^2 = J(J+1)$$

In the vibrational term $G(V)$, it is ordinarily only necessary to retain the first anharmonic parameter, $\omega_e x_e$, in addition to the harmonic vibration frequency, ω_e; in the rotational term $F(J)$, usually only the vibration-rotation interaction constant, α_e,

and centrifugal distortion constant, D_e, are needed in addition to the rotational constant, B_e. The following relations hold to a very good approximation.[3,4]

$$4\pi^2\mu\omega_e^2 r_e^2 = F_2 r_e^2 = 2a_0 \tag{9}$$

$$B_e = \frac{(h/8\pi^2)}{\mu r_e^2} \tag{10}$$

$$\alpha_e = -\frac{6B_e^2}{\omega_e}(1+a_1) \tag{11}$$

$$\omega_e x_e = -\frac{3B_e}{2}(a_2 - \frac{5}{4}a_1^2) \tag{12}$$

$$D_e = -\frac{4B_e^3}{\omega_e^2} \tag{13}$$

From these are obtained the working equations for force constant calculations:

$$F_2 = (5.8893 \times 10^{-7})\mu\omega_e^2 \tag{14}$$

$$F_3 = a_1(F_2/r_e) \tag{15}$$

$$F_4 = a_2(F_2/r_e^2) \tag{16}$$

$$-a_1 = 1 + (\alpha_e\omega_e/6B_e^2) \tag{17}$$

$$a_2 = (5/4)a_1^2 - (2/3)(\omega_e x_e/B_e) \tag{18}$$

The bond length is calculated from

$$I_e = \mu r_e^2 = 16.863/B_e \tag{19}$$

The system of units used is:

spectroscopic constants, cm^{-1}

$B_e, \alpha_e, \omega_e, \omega_e x_e$

reduced mass, μ	gm/mole
bond length, r_e	Å
force constants,	
F_2	10^5 dynes/cm
F_3	10^{13} dynes/cm^2
F_4	10^{21} dynes/cm^3 ;

The tables given in this report were prepared in the course of an empirical study of the dependence of the force constants on bond length, described in a previous report,[5] UCRL-9537.

Table I supplements the very extensive tabulation of spectroscopic parameters given by Herzberg.[1] Molecules are listed according to the rows of the periodic table to which the atoms belong. Data are given for all reasonably well established electronic states (not already listed in Herzberg's table) for which both vibrational and rotational parameters have been determined. An attempt was made to include all new and revised parameters published up to December, 1960. However, it should perhaps be emphasized that Table I is a much less complete and critical compilation than Herzberg's. The bibliography is not intended to be exhaustive, and much additional spectroscopic information has not been abstracted. We have not attempted to review the data critically or to apply various corrections, as this was unnecessary for our study. Herzberg is preparing a revised edition of his table.

Table II lists values of the force constants a_1, a_2, F_2, F_3, and F_4 derived from the data given in Herzberg's table and

in Table I. The relations (14)-(19) were used throughout. Since these relations, as well as (9)-(13), neglect terms of order B_e^2/ω_e^2, small corrections[3,4] should have been included for the hydride molecules. These corrections are quite awkward to apply and require one to estimate the values of a_n constants with $n > 2$. When this was done by using a Morse potential function,[4] the corrections to the force constants were insignificant for our purposes. Also, the corrections generally failed to bring the force constants for hydrogen and deuterium isotopes into agreement. It was therefore decided to omit the corrections in the final tabulations, and to list separately values of the uncorrected force constants for the hydrogen and deuterium isotopes.

As shown in UCRL-9537, the force constants F_n are approximately exponential functions of internuclear distance. Table III gives the parameters a_{ij} and b_{ij} in the function

$$(-1)^n F_n = 10^{-(r_e - a_{ij})/b_{ij}}$$

These values were obtained by fitting straight lines to semi-logrithmic graphs of the data of Table II. As indicated, each pair of parameters refers to a given type of force constant ($n = 2,3,4$) for bonds between atoms from rows i and j of the periodic table. It was found that molecules containing transition metals bonded to hydrogen or first row atoms required parameters considerably different from those for other molecules in the same row, and consequently the parameters for molecules

with transition metals are listed separately at the bottom of Table III. In determining the parameters, data for ionic and excited electronic states were included but assigned one-fourth the weight of the data for ground states. For many of the anharmonic force constants the uncertainty is several per cent or more; data for which the uncertainty is greater than 25% were excluded.

In order to indicate the accuracy that can be expected in using Table III, the average percentage deviation between observed and calculated force constants is given for each of the families of molecules considered. The average deviations were computed just for the ground electronic states. A few cases in which large, atypical deviations occurred were not included in the averages but are listed separately. To obtain the most reliable estimates of force constants for a new molecule or a new electronic state, one should make direct use of the data for related molecules given in Table II, restricting comparisons to molecules in which the bond character is similar. Although it has been most convenient to organize the data according to rows of the periodic table, smooth trends are also usually found for molecules whose atoms belong to corresponding columns.

Since the force constants have an approximately exponential dependence on the internuclear distance, the relations of Table III are less accurate when used to predict force constants from known distances than when used to estimate distances from known force constants. The relative error to be expected in the prediction of a distance may be approximated by multiplying the

average deviation listed under Table III by the factor b_{ij}/r_e; this varies from about one-half to one-sixth for the various families of molecules. Thus, Table III can sometimes provide useful estimates of bond distances of electronic states for which a vibrational analysis has been made but not a rotational analysis.

Table IV lists some force constants for polyatomic molecules. The predicted values of the cubic force constants were obtained from the relations of Table III. The experimental values were derived from vibration-rotation interaction constants given in the references cited in the bibliography. The methods used were similar to those described by

D. M. Dennison, Rev. Mod. Phys. 12, 175 (1940).

B. T. Darling and D. M. Dennison, Phys. Rev. 57, 128 (1940).

J. Pliva, Coll. Czechoslav. Chem. Sommuns. 23, 777 (1958).

A valence force field has been assumed, in which the part of the vibrational potential due to the stretching of a particular bond has the form (n = 2,3):

$$2U = \Sigma_n F_n (r-r_e)^n + \text{interaction terms}$$

Except for CO_2 and H_2O, the interaction terms had to be neglected in deriving the cubic force constants. Further uncertainties arise from the experimental error in the vibration-rotation parameters and normal coordinates which enter into the calculations. Although it seems unlikely that the experimental

cubic constants are in error by as much as 20%, there is no satisfactory way to make a more specific error estimate.

Tables of quadratic force constants for bond stretching in polyatomic molecules are given by

Wilson, Decius, and Cross, Molecular Vibrations (McGraw-Hill, New York, 1955), p. 175.

Herzberg, Infrared and Raman Spectra (D. Van Nostrand, New York, 1945), p. 193.

Acknowledgments

We wish to thank Patricia Kurth, Pearl Keeley, Nancy Monroe, and David Ham for their aid in the preparation of these tables.

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1. G. Herzberg, Spectra of Diatomic Molecules (D. Van Nostrand Co., New York, 1950).
2. A. G. Gaydon, Dissociation Energies and Spectra of Diatomic Molecules (Chapman and Hall, London, 2nd Ed., 1953).
3. C. H. Townes and A. L. Schawlow, Microwave Spectroscopy (McGraw-Hill, New York, 1955).
4. J. L. Dunham, Phys. Rev. 41, 721 (1932).
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Table I. Vibrational and Rotational Parameters of Diatomic Molecules

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
			H-1			
LiH μ = 0.881506						
$B^1\Pi$	2.378	3.383	0.986	215.5	42.4	69
LiD μ = 1.56535						
$B^1\Pi$	2.376	1.908	0.427	177.28	29.13	69
CH μ = 0.930024						
$^2\Pi$	1.1202	14.448	0.530	2868.5	64.4	54
$^2\Delta$	1.1020	14.930	0.690	2943.0	99.3	54
HF^+ μ = 0.957347						
$B^2\Sigma^+$	2.092	4.027_7	0.0216	1158.4	17.2	59
$A^2\Sigma^+$	1.076	15.212	0.6746	2977.6	111.91	59
NH μ = 0.940447						
$X^3\Sigma^-$	1.037	[16.3454]	[0.646]	[3125.6]		76
$A^3\Pi_i$	1.036	[16.322_1]	[0.744]	[3034.0]		76
			H-2			
PH^+ μ = 0.97636						
$^2\Delta$	1.548_8	7.1955	0.4245	1398.76	-	63
$X^2\Pi$	1.425_1	8.505_1	0.240_1	[2299.60]	-	63
SiH μ = 0.973080						
$^2\Delta$	1.523	7.470	0.347	1858.13	98.73	58
$X^2\Pi$	1.521	7.498	0.214	2042.47	35.67	58
AlD μ = 1.87478						
$C^3\Pi_r$	1.593	3.545	0.096	1260	-	27

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
			H-3			
GeH μ = 1.14768						
$^2\Delta'$	1.611	6.551	0.620	1227	-	28
$X^2\Pi''$	1.591	6.720	0.174	1876	-	28
$(HBr)^+$ μ = 0.99558						
$X^2\Pi_i$	1.448	8.072_0	0.236_3	2450	(50)	25
$A^2\Sigma^+$	1.684	5.970_2	0.247_6	1409	(40)	25
			1-1			
BeO μ = 5.76612						
$'\Sigma^+$	1.3308	1.6510	0.0190	1487.19	11.731	79
F_2 μ = 9.50227						
$'\Sigma_g^+$	1.412	0.8901	(0.0146)	919.0	(13.6)	79
BN μ = 6.16500						
$(X)^3\Pi$	1.281	1.682	0.025	1522.0	12.4	7,80
BF μ = 6.97245						
$X'\Sigma^+$	1.265_2	1.510_7	0.0165	1402.1_3	11.8_4	65
$A'\Pi$	1.3047	1.4206	0.0165	1264.9_6	12.5_3	65
CF μ = 7.35693						
$X^2\Pi$	1.2708	1.4190	0.019_0	$1308._4$	10.8_6	11
B?	1.318	1.320	0.025	1191.0	19.4	11
$A^2\Sigma^+$	1.1516	1.727_7	0.0260	1764	22	11

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
CN^+ μ = 6.46427						
$f'\Sigma$	1.171	1.903	0.032	2670.5	46.9	35
$a'\Sigma$	1.1727	1.8964	0.0188	2033.05	16.14	35
$c'\Sigma$	(1.363)	(1.403)	(0.002)	1265	(11)	35
CN μ = 6.46427						
$J^2\Delta_i$	1.414	1.305_6	0.020_7	1121.76	14.203	53
LiF μ = 5.1254						
$X'\Sigma$	1.545	1.378	0.01971	906.2	7.90	86

$Cl^{35}F$ μ = 12.31420						
$X^1\Sigma$	1.62811	0.51651	0.0043588	786.34	6.23	21
MgF μ = 10.60470						
$^2\Sigma$	1.75_0	(0.516)	(0.004)	717.0	3.84	79
ClO μ = 11.026						
$^2\Pi$	1.54	(0.646)	(0.007)	868	7.5	79
AlF μ = 11.1521						
$X'\Sigma^+$	1.654_7	0.55_{28}	0.004_{83}	801.95	4.7_0	68
$B'\Sigma^+$	1.6170	0.578_{34}	0.004_{71}	866.60	7.4_5	68
$A'\Pi$	1.64_9	0.5563_9	0.0051_6	804.69	6.3525	52
NS μ = 9.74115						
$X^2\Pi$	1.495_7	0.77364	0.0061_2	1204.14	-	16

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
SiO	μ = 10.18013					
$A^1\Pi$	1.620	0.6312_8	0.00695	852.7_1	6.4_4	30
$X^1\Sigma$	1.509	0.7272_9	0.00508	1241.4_4	5.9_2	30
MgO	μ = 9.59888					
$^1\Sigma^{**}$	1.737	0.5822	0.0045	824.0_8	4.7_6	2
$^1\Pi$	1.864	0.5056	0.0046	664.4_4	3.9_1	2
$(X)'\Sigma^+$	1.749	0.5743	0.0050	785.0_6	5.1_8	2
AlO	μ = 10.0452					
$^2\Sigma''$	1.6176	0.6413_6	0.0058_0	979.23	6.97	62
$^2\Sigma'$	1.6668	0.6040_8	0.0044_7	870.05	3.5_2	62
BS	μ = 8.19196					
$A^2\Pi$	1.8177	0.6229_1	0.0059_2	748.73	4.62	17
$X^2\Sigma$	1.6091	0.7948_9	0.0060_5	1180.17	6.31	17
PO	μ = 10.55138					
E	1.420	0.792	0.008	(1457.6)	-	47
B	1.434	0.7769	0.0095	1166.2	14.10	47
$A^2\Sigma^+$	1.403	0.8121	0.0056	1391.0	7.65	47
$X^2\Pi$	1.447	0.7629	0.0055	1232.5	6.50	47
SiF	μ = 11.3187					
?	1.549	0.621	0.00_2	1005.5	5.2_2	13

1-3

$Br^{79}F$	μ = 15.31710					
$X^1\Sigma^+$	1.75555	0.357165	0.005214	671.9	3.0	21

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
CSe^{80}	μ = 10.4366					
$X^1\Sigma^+$	1.66_9	0.58_0	0.004_0	1035.9	4.8_8	31
$Ga^{69}F$	μ = 14.8980					
$C^1\Pi$	1.778	0.358_{05}	0.0053_5	542.35	9.5_5	57
$B^3\Pi_1$	1.745_3	0.3715_4	0.0030_2	662.1	1.45	57
$A^3\Pi_{0+}$	1.747_6	0.3705_3	0.0030_2	663.0_2	2.18	57
$X^1\Sigma^+$	1.775_4	0.35905	0.0028_2	622.2	3.2	57
VO	μ = 12.1768					
$(A^2\Delta)$	1.672	0.4953	0.0035	865.9	(6.6)	60
$(X^2\Delta)$	1.589	0.5480	0.0034	1011.56	4.97	60
CaO	μ = 11.4265					
$B^1\Pi$	1.950	0.388_2	0.005_5	580	-	39
$C^1\Sigma$	1.989	0.3731	0.0032	560.9	4.0	39
$A^1\Sigma$	1.906	0.4063	0.0014_1	(716)	(1.6)	8
$(X)^1\Sigma$	1.822	0.4444_7	0.0033_5	732.1	4.81	8
LiBr	μ = 6.4517					
$X^1\Sigma$	2.1704	0.5548	0.005633	563.2	3.53	36, 83
KF	μ = 12.7897					
$X^1\Sigma$	2.17144	0.27994	0.002335			82

1-4

InF	μ = 16.30808					
$C^1\Pi$	1.97_0	0.2664	0.005_0	463.9	7.35	45
$B^3\Pi_1$	1.943_8	0.27378	0.0020_4	572.2_5	2.63	45
$A^3\Pi_{0+}$	1.944_8	0.2733_6	0.0020_2	575.2	3.67_8	45
$X^1\Sigma^+$	1.984_7	0.2624_7	0.0018_6	535.3_5	2.63_5	45

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
SrO	μ = 13.5302					
$^1\Pi$	2.060	0.2936_1	0.0013_2	520	-	29
$A^1\Sigma$	2.027	0.3047_1	0.0011_2	(619.6)	(0.9)	5
$C^1\Sigma$	2.132	0.2742	0.0021	480.2	(2.6)	37
$X'^1\Sigma$	1.923	0.3377_9	0.0020_4	635.49	3.96	61, 29
$Zr^{90}O^{16}$	μ = 13.5836					
$A''(^1\Sigma)$	1.725	0.4167	(0.0012)	938.1	1.80	4, 56
$A'(^1\Sigma)$	1.764	0.3986	0.0021	839.2	2.56	4, 56
$B'(^1\Sigma)$	1.772	0.3951	0.0019	843.2_7	3.0_4	51, 3
$B''(^1\Sigma)$	1.711	0.4241	0.0023	978.07	5.04	51, 3
$C^3\Delta$	1.775	0.3927	0.0021	820.58	3.31	38,3,4
$A^3\Phi$	1.752	0.4035	0.0021	856.97	3.37	38
$X^3\Delta$	1.728	0.4147	0.0021	937.20	3.35	38
AgO	μ = 13.9340					
$X^2\Pi_{3/2}$	1.998	0.3035	0.0025_5	490.6	2.9	41
$X^2\Pi_{1/2}$	2.003	0.3020	0.0025	490.2	-	41
NbO	μ = 13.64998					
$A^2\Delta'$	1.757	0.4001	0.0019	850.48	3.37	42
$X^2\Delta''$	1.691	0.4321	0.0021	989.0	3.83	42
$Sn^{120}O^{16}$	μ = 14.0999					
$A^1\Pi$	1.950	0.31455	0.0025	~580	3.08	78
$X^1\Sigma^+$	1.832	0.3561	0.0022	822.1	3.73	78
$I^{127}O^{16}$	μ = 14.2090					
$A^2\Pi_{3/2}$	2.0723	0.2763_5	0.0027_3	514.5_7	5.5_2	81

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
$X^2\Pi_{3/2}$	1.8676	0.34026	0.00269_6	681.4_7	4.2_9	81
LiI	μ = 6.6505					
$X^1\Sigma$	2.3919	0.44320	0.004090	498.2	3.3_9	36,83
RbF	μ = 15.5483					
$X^1\Sigma$	2.2655	0.21066	0.001522			75
			1-5			
$Tl^{205}F$	μ = 17.3923					
$X^1\Sigma^+$	2.0844	0.223153	0.001500	475.00	1.89	7, 70
TaO	μ = 14.7000					
$c^2\Delta$	1.743	0.3775	0.0019	903.01	4.15	66
$b^2\Pi$	1.744	0.3772	0.0019	897.3	4.1	66
$(X)a^2\Delta$	1.687	0.4029	0.0020	1031.7	5	66
BaO	μ = 14.3311					
$(^1\Sigma?)$	2.2847	0.2254	0.0013_5	450.4	2.9	9
$^1\Sigma$	2.133	0.2584	0.0011_1	(500)	(1.6)	9
$(X)^1\Sigma$	1.940	0.3124_9	0.00130	669.8_1	2.05_4	9
CsF	μ = 16.6276					
$X^1\Sigma$	2.3453	0.18437	0.001105	385	1.2_3	36
			2-2			
MgCl	μ = 14.23132					
$^2\Sigma$	2.18	(0.245)	(0.001)	465.4	2.05	79
SiS	μ = 14.92589					
$^3\Sigma^-$	2.258	0.221_6	0.002_9	≥ 407.2	1.7_7	55
$^1\Sigma^-$	2.301	0.213_3	0.001_8	≥ 404.9	1.1_8	55

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
$D^1\Pi$	2.0589	0.2664_7	0.0021_6	513.1_2	2.9_3	22
$^1\Pi$ or $^1\Delta$	2.2313	0.2269	0.0028	439.9	3.9_7	55
$X^1\Sigma^+$	1.928_8	0.30363	0.014_9	749.6_9	2.58	22
P_2^+	μ = 15.49221					
$b^2\Pi$	1.9902	0.2154	0.0017	436.12	2.54	64
$a^2\Pi$	2.2480	0.2748	0.0017	666.48	2.63	64
$X^2\Sigma_g^+$	1.896	[0.3027]	[0.0021]	[733.4]		74
P_2	μ = 15.49221					
$B^1\Sigma_u^+$	2.122	0.24166	0.00165	475.24	2.633	72
$A^1\Pi_g$	1.9883	0.27520	0.00169	618.88	(2.97)	72
$X^1\Sigma_g$	1.8931	0.30359	0.001477	780.89	2.820	72
Si_2	μ = 14.034					
$H^3\Sigma_u^-$	2.663	0.1699	0.00135	271.32	1.99	46,72
$D^3\Pi_g$	2.155	0.2596	0.00155	547.94	2.43	46,72
$(X)^3\Sigma_g^-$	2.252	0.2376	0.00135	506.72	1.97	46,72
AlCl	μ = 15.2350					
$A^3\Pi$	2.1041	0.250	0.002	524.35	2.175	15
NaCl	μ = 13.9517					
$X^1\Sigma$	2.3606	0.21805	0.001610	366.1	(2.05)	36,67
			2-3			
$Ga^{69}Cl^{35}$	μ = 23.2069					
$X^1\Sigma^+$	2.2017	0.149894	0.0007762	365.0	1.1	70
$Br^{79}Cl^{35}$	μ = 24.23944					
$X^1\Sigma^+$	2.138	0.152469	0.0007745	[430]	-	10

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
AlBr	μ = 20.1129					
$a^3\Pi_1$	2.2610	0.164	0.001	410.32	1.75	15
$CaCl^{35}$	μ = 18.6804					
$C^2\Pi$	2.5160	0.14268	0.000747	336.0	1.4	84
$X^2\Sigma^+$	2.439_0	0.15156	0.00078_3	369.0	1.31	84
NaBr	μ = 17.8589					
$X^1\Sigma$	2.5020	0.1495	0.0009394	302.1	(1.50)	36,67
KCl	μ = 18.6009					
$X^1\Sigma$	2.6666	0.1285	0.0007893	281	(1.30)	36,67
			2-4			
$In^{115}Cl^{35}$	μ = 26.8179					
$X^1\Sigma^+$	2.4011	0.109058	0.0005120	317.4	1.01	70
$I^{127}Cl^{35}$	μ = 27.42341					
$X^1\Sigma^+$	2.3207	0.114162	0.000536	384.18	1.465	21
NaI	μ = 19.4699					
$X^1\Sigma$	2.7115	0.1177	0.0006480	258	(1.08)	36,67
RbCl	μ = 25.0699					
$X^1\Sigma$	2.7868	0.08764	0.0004536	228	(0.92)	36,67
			2-5			
$Tl^{205}Cl^{35}$	μ = 29.869					
$X^1\Sigma^+$	2.4848	0.0913981	0.0003969	287.47	1.24	70
CsCl	μ = 28.0005					
$X^1\Sigma$	2.9062	0.07204	0.0003362	209	(0.75)	36,67

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
			3-3			
$Ga^{69}Br^{79}$	μ = 36.8039					
$X^1\Sigma^+$	2.3525	0.0827902	0.0003249	263.0	0.81	70
KBr	μ = 26.2609					
$X^1\Sigma$	2.8207	0.08117	0.0004025	213	(0.80)	36,67
			3-4			
$In^{115}Br^{79}$	μ = 46.9654					
$X^1\Sigma^+$	2.5432	0.0557098	0.0001903	221.0	0.65	70
$Ga^{69}I^{127}$	μ = 44.682					
$X^1\Sigma^+$	2.5747	0.0569346	0.0001891	216.4	0.5	70
KI	μ = 29.8987					
$X^1\Sigma$	3.0478	0.060713	0.0002666	(173)		36,67
RbBr	μ = 41.3102					
$X^1\Sigma$	2.9448	0.04753	0.0001861	(166)		36.67
			3-5			
$Tl^{205}Br^{79}$	μ = 56.9982					
$X^1\Sigma^+$	2.6181	0.431595	0.0001310	192.1	0.39	70
CsBr	μ = 49.9194					
$X^1\Sigma$	3.0720	0.035790	0.0001225	(139)		36,67
			4-4			
$In^{115}I^{127}$	μ = 60.3207					
$X^1\Sigma^+$	2.7539	0.0368571	0.0001040	177.1	0.4	70
RbI	μ = 51.0885					
$X^1\Sigma$	3.1769	0.032707	0.0001089	(128)		36,67

State	r_e	B_e	α_e	ω_e	$\omega_e x_e$	Ref.
$Tl^{205}I^{127}$	μ = 78.4036					
$X^1\Sigma^+$	2.8135	0.0271681	0.00006621 (150)			70,7
CsI	μ = 65.9389					
$X^1\Sigma$	3.3150	0.02363	0.00006818 (101)			36,67

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Table II. Quadratic, Cubic, and Quartic Vibrational Force Constants of Diatomic Molecules

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
			H-1				
HF	$X^1\Sigma^+$	0.9171	2.21	3.24	9.657	23.3	37.2
DF	$X\Sigma^+$	0.9170	2.29	3.78	9.644	24.1	43.3
$O^{16}D$	$A^2\Sigma^+$	1.012	2.47		5.672	13.8	
	$X^2\Pi_i$	0.9699	2.31	3.74	7.802	18.6	31.0
$O^{16}H$	$A^2\Sigma^+$	1.0121	2.42		5.650	13.5	
	$X^2\Pi$	0.9706	2.25	3.39	7.793	18.1	28.1
$(O^{16}H)^+$	$A^3\Pi_i$	1.1368	2.48		2.203	4.69	
	$X^3\Sigma^-$	1.0289	2.28		4.877	10.8	16.8
$N^{14}H$	$C^1\Pi$	1.125	3.45		2.487	7.62	
	$A^3\Pi_i$	1.037	2.47		6.032	14.3	
	$a^1\Delta$	1.043	1.33		5.622	7.19	
	$X^3\Sigma^-$	1.038	2.27		6.032	13.2	
$(HF^{19})^+$	$B^2\Sigma^+$	2.092	1.26	-0.13	0.7566	0.455	-0.22
	$A^2\Sigma^+$	1.076	2.45	2.58	4.999	11.4	11.1
$C^{12}D$	$C^2\Sigma^+$	1.1137	2.57		4.368	10.1	
	$B^2\Sigma^-$	1.1674	4.09		3.321	11.7	
	$A^2\Delta$	1.1031	2.44		4.672	10.3	
	$X^2\Pi$	1.1188	2.22	3.19	4.485	8.90	11.4
$C^{12}H$	$C^2\Sigma^+$	1.1132	2.64		4.368	10.3	
	$B^2\Sigma^-$	1.1861	2.24		3.541	6.68	
	$A^2\Delta$	1.1020	2.52	3.49	4.744	10.8	13.6
	$X^2\Pi$	1.1202	2.21	3.15	4.507	8.91	11.3
$(C^{12}H)^+$	$A^1\Pi$	1.2344	3.04	5.73	1.874	4.62	7.05
	$X^1\Sigma^+$	1.1308	2.11		4.111	7.67	
$B^{11}D$	$A^1\Pi$	1.2198	2.86		2.899	6.79	
	$X^1\Sigma^+$	1.2311	2.15	3.05	3.178	5.56	6.39

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$B^{11}H$	$B^1\Sigma^+$	1.2149	2.49		3.133	6.43	
	$A^1\Pi$	1.2257	2.38		2.988	5.80	
	$X^1\Sigma^+$	1.2325	2.13	2.93	3.045	5.25	5.86
$(Be^9D)^+$	$A^1\Sigma^+$	1.6057	1.67		1.166	1.21	
	$X^1\Sigma^+$	1.3113	1.95	2.33	2.633	3.93	3.57
(Be^9H^+)	$A^1\Sigma^+$	1.6089	1.60		1.164	1.15	
	$X^1\Sigma^+$	1.3122	1.93	2.21	2.636	3.88	3.39
Be^9H	$A^2\Pi$	1.3327	2.04		2.327	3.57	
	$X^2\Sigma^+$	1.3431	1.97	2.55	2.263	3.32	3.20
Li^7D	$B^1\Pi$	2.376	4.46	14.7	0.02897	0.0544	0.0757
	$A^1\Sigma^+$	2.5859	-1.17		0.3016	-0.136	
	$X^1\Sigma^+$	1.5949	1.91	2.46	1.0263	1.23	0.993
Li^7H	$B^1\Pi$	2.378	4.09	12.6	0.02411	0.0415	0.0537
	$A^1\Sigma^+$	2.5963	-1.39		0.2853	-0.152	
	$X^1\Sigma^+$	1.5953	1.88	2.38	1.0258	1.21	0.961
			H-2				
HCl^{35}	$X^1\Sigma^+$	1.2746	2.34	3.57	5.158	9.47	11.4
DCl^{35}	$X^1\Sigma^+$	1.2749	2.98		4.904	11.5	
$(HCl^{35})^+$	$A^2\Sigma^+$	1.5138	2.62		1.488	2.58	
	$X^2\Pi_i$	1.3153	2.43	3.22	4.131	7.65	7.70
$(DCl^{35})^+$	$A^2\Sigma^+$	1.5149	2.47		1.386	2.27	
	$X^2\Pi_i$	1.3153	2.39		3.898	7.08	
$Si^{28}H$	$A^2\Delta$	1.523	2.93	1.89	1.979	3.80	1.61
	$X^2\Pi_r$	1.521	2.30	3.42	2.964	4.47	4.38
$(P^{31}H)^+$	$^2\Pi$	1.4251	2.27		3.041	4.85	
	$^2\Delta$	1.5488	2.91		1.125	2.11	
$(Al^{27}H)^+$	$A^2\Pi_r$	1.5913	2.99		1.759	3.30	
	$X^2\Sigma^+$	1.6016	3.34		1.484	3.09	

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$Al^{27}D$	$C^3\Pi_r$	1.593	2.60		1.753	2.87	
	$C^1\Sigma^+$	1.617	3.49		1.113	2.40	
	$A^1\Pi$	1.667	2.75		1.137	1.88	
	$X^1\Sigma^+$	1.6456	2.28	3.45	1.622	2.28	2.07
$Al^{27}H$	$C^1\Sigma^+$	1.613	4.22		0.8314	2.17	
	$A^1\Pi$	1.6466	4.29		0.6714	1.75	
	$X^1\Sigma^+$	1.64822	2.28	3.44	1.620	2.24	2.05
$(Mg^{24}H)^+$	$A^1\Sigma^+$	2.006	1.77		0.731	0.643	
	$X^1\Sigma^+$	1.649	2.42	4.16	1.638	2.40	2.50
$(Mg^{24}D)^+$	$A^1\Sigma^+$	2.007	1.62		0.731	0.5891	
	$X^1\Sigma^+$	1.653	2.19	2.70	1.647	2.1782	1.63
$Mg^{24}D$	$C^2\Pi$	1.661	3.75		1.519	3.43	
	$A^2\Pi_r$	1.6797	2.25		1.461	1.96	
	$X^2\Sigma^+$	1.7301	2.28	2.95	1.272	1.67	1.25
$Mg^{24}H$	$C^2\Pi$	1.682	2.10	-0.6	1.725	2.15	-3.68
	$A^2\Pi_r$	1.6795	2.33		1.479	2.05	
	$X^2\Sigma^+$	1.7306	2.23	2.60	1.275	1.64	1.11
$Na^{23}D$	$X^1\Sigma^+$	1.8865	2.09		0.745	0.827	
$Na^{23}H$	$A^1\Sigma^+$	3.208	1.32	0.031	5.487	2.25	0.0166
	$X^1\Sigma^+$	1.8873	2.10	2.83	0.782	0.870	0.621
			H-3				
HBr	$X^1\Sigma^+$	1.4138	2.39	3.59	4.116	6.96	7.41
$(HBr)^+$	$A^2\Sigma^+$	1.684	2.63	4.19	1.170	1.83	1.73
	$X^2\Pi_i$	1.448	2.48	3.56	3.519	6.03	5.98
$Cu^{63}H$	$D^1\Pi$	1.48	2.51		1.902	3.22	
	$B^1\Sigma^+$	1.606	2.73		1.426	2.42	
	$A^1\Sigma^+$	1.572	2.58		1.686	2.76	
	$X^1\Sigma^+$	1.463	2.28	3.38	2.200	3.43	3.47
NiH	$X^2\Delta_{\frac{5}{2}}$	1.4746	2.30		2.166	3.38	

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$Ge^{74}H$	$^2\Delta$	1.611	3.95		1.018	2.50	
	$X^2\Pi$	1.591	2.21		2.379	3.30	
ZnH	$A^2\Pi_r$	1.5108	2.39		2.134	3.38	
	$X^2\Sigma^+$	1.5945	2.50	2.32	1.511	2.37	1.38
$Mn^{55}H$	$X^7\Sigma$	1.7308	2.24		1.295	1.67	
$Ca^{40}H$	$D^2\Sigma$	2.62	1.31		0.765	0.381	
	$B^2\Sigma$	1.954	1.62		0.956	0.791	
	$A^2\Pi_r$	1.99	2.18		1.029	1.13	
	$X^2\Sigma$	2.0020	2.14	2.68	0.977	1.04	0.654
$K^{39}H$	$X^1\Sigma^+$	2.244	1.92	1.90	0.562	0.488	0.211
$K^{39}D$	$X^1\Sigma^+$	2.298	2.19	2.9	0.562	0.537	0.31
			H-4				
HI^{127}	$X^1\Sigma^+$	1.6041	2.64	4.68	3.142	5.17	5.71
AgH	$A^1\Sigma^+$	1.6415	2.43		1.628	2.41	
	$X^1\Sigma^+$	1.6174	3.45	11.3	1.822	3.89	7.84
CaH	$A^2\Pi$	1.6633	2.54		1.819	2.78	
	$X^2\Sigma^+$	1.7617	2.76	3.83	1.205	1.89	1.49
$In^{115}H$	$B^1\Pi$	1.7610	3.05		1.308	2.27	
	$A^1\Sigma^+$	1.7735	3.74		1.258	2.64	
	$X^1\Sigma^+$	1.8376	2.43	4.07	1.280	1.69	1.54
SrH	$C^2\Sigma^+$	2.054	2.84		1.065	1.48	
	$D^2\Sigma^+$	2.964	2.10		0.604	0.43	
	$X^2\Sigma^+$	2.1455	2.21	3.03	0.854	0.880	0.562
RbH	$A^1\Sigma^+$	3.708	-1.62		0.0351	-0.0154	
	$X^1\Sigma^+$	2.367	2.23	3.11	0.5149	0.486	0.286
			H-5				
$Au^{197}H$	$A^1\Sigma^+$	1.67284	2.92		1.647	2.87	
	$X^1\Sigma^+$	1.52373	2.57	4.26	3.138	5.284	5.75

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$(HgD)^+$	$A^1\Sigma^+$	1.692	2.63	3.73	1.554	2.41	2.02
	$X^1\Sigma^+$	1.5937	2.59	3.73	2.443	3.97	3.59
$(HgH)^+$	$A^1\Sigma^+$	1.6922	2.63	3.76	1.552	2.41	2.04
	$X^1\Sigma^+$	1.5943	2.60	4.85	2.444	3.98	4.68
HgD	$X^2\Sigma$	1.7378	3.400	2.55	1.163	2.762	0.981
HgH	$A^2\Pi_{\frac{3}{2}}$	1.5803	2.63		2.524	4.20	
	$A^2\Pi_{\frac{1}{2}}$	1.5859	2.87		2.521	4.56	
	$X^2\Sigma^+$	1.7404	3.29	3.59	1.137	2.15	1.35
$Bi^{209}H$	$C^1\Sigma$	1.96	2.26		1.020	1.18	
	BO^+	1.780	2.90		1.764	2.87	
	A(1)	1.788	2.62		1.788	2.62	
	$X(O^+)$	1.809	2.59	4.27	1.705	2.44	2.23
$Bi^{209}D$	$B(O^+)$	1.779	2.85	3.90	1.792	2.87	2.21
	$X(O^+)$	1.805	2.61	4.37	1.708	2.47	2.29
TlH	EO^+	2.319	7.13		0.915	2.82	
	DO^+	2.219	8.30		0.866	3.24	
	CO^+	1.944	12.34		0.952	6.05	
	$X^1\Sigma^+$	1.870	2.46	4.39	1.143	1.50	1.43
BaH	$E^2\Pi$	2.18	2.25		0.893	0.92	
	$C^2\Sigma$	2.18	1.79		1.032	0.85	
	$B^2\Sigma$	2.27	2.19		0.698	0.67	
	$X^2\Sigma^+$	2.23	2.12	2.46	0.810	0.768	0.218
$Cs^{133}H$	$A^1\Sigma^+$	3.87	0.504	35.2	0.0245	0.00320	0.0579
	$X^1\Sigma^+$	2.49	2.15	2.69	0.4675	0.404	0.419
			1-1				
N_2^{14}	$C^3\Pi_u$	1.1483	3.00		17.08	44.7	
	$B^3\Pi_g$	1.2123	2.98		12.40	30.5	
	$A^3\Sigma_u^+$	1.293	2.53		8.798	17.2	
	$b^{11}\Sigma_u^+$	1.450	1.19		0.233	0.191	
	$a^1\Pi_g$	1.213	3.32		11.81	32.3	

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
	$X^1\Sigma_g^+$	1.094	2.82	5.15	22.96	59.2	99.6
$(C^{12}O^{16})^+$	$B^2\Sigma^+$	1.16868	3.70		12.147	38.5	
	$A^2\Pi_i$	1.24368	3.00		9.855	23.8	
	$X^2\Sigma^+$	1.11506	2.79	4.62	19.803	48.0	
$(N_2^{14})^+$	$B^2\Sigma_u^+$	1.075	2.81		24.153	63.2	
	$X^2\Sigma_g^+$	1.1162	2.97	5.47	20.094	53.5	
$(O_2^{16})^+$	$b^4\Sigma_g^-$	1.27953	3.66		6.748	19.3	
	$A^2\Pi_u$	1.4089	2.54		3.816	6.87	
	$a^4\Pi_u$	1.38126	3.23		5.054	11.8	
	$X^2\Pi_g$	1.1227	3.22	6.36	16.59	47.6	83.7
$C^{12}O^{16}$	$d^3\Pi_i$	1.3960	3.03		5.229	11.3	
	$b^3\Sigma^+$	1.088	3.81		19.51	68.3	
	$a'^3\Sigma^+$	1.359	2.83		5.988	12.5	
	$a^3\Pi_r$	1.2093	2.98		12.22	30.1	
	$B^1\Sigma^+$	1.120	3.44		17.51	53.7	
	$A^1\Pi$	1.2351	3.09		9.28	23.2	
	$X^1\Sigma^+$	1.12819	2.70	4.43	19.02	45.5	66.3
$N^{14}O^{16}$	$E^2\Sigma^+$	1.0661	2.83		24.78	65.6	
	$B^2\Pi_r^*$	1.385	3.36		4.743	11.5	
	$B^2\Pi_r$	1.448	2.73		4.730	8.92	
	$A^2\Sigma^+$	1.0637	2.63		24.734	61.1	
	$X^2\Pi$	1.1508	2.94	5.37	15.944	41.3	64.6
$C^{12}N^{14}$	$J^2\Delta_i$	1.414	3.27	6.12	4.791	11.1	14.7
	$B^2\Sigma^+$	1.1506	3.06		17.830	47.4	
	$A^2\Pi_i$	1.2327	2.79		12.533	28.4	
	$X^2\Sigma^+$	1.1718	2.66	4.22	16.29	37.0	50.1
$(C^{12}N^{14})^+$	$f^1\Sigma$	1.1727	4.93	14.0	27.150	114.	277.
	$c^1\Sigma$	1.363	1.21		6.092	5.4	
	$a^1\Sigma$	1.1727	2.77	3.84	15.736	13.2	46.5
$B^{11}O^{16}$	$A^2\Pi_i$	1.3524	3.06		6.106	13.8	
	$X^2\Sigma^+$	1.2049	2.63	4.63	13.656	29.9	40.1

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
O_2^{16}	$B^3\Sigma_u^-$	1.604	2.91		2.311	4.21	
	$b^1\Sigma_g^+$	1.22675		3.21		9.671	25.3
	$a^1\Delta_g$	1.2155	3.14		10.73	27.5	
	$X^3\Sigma_g^-$	1.20740	2.99	5.61	11.76	29.1	45.3
$B^{11}F^{19}$	$b^3\Sigma$	1.2166	3.09		10.93	27.8	
	$a^3\Pi$	1.3086	2.98		7.1943	16.4	
	$A^1\Pi$	1.3047	2.72	3.49	6.571	11.9	28.6
	$X^1\Sigma^+$	1.2652	2.69	3.82	8.073	17.2	19.3
$C^{12}F^{19}$	B	1.318	3.85	8.71	6.146	17.9	30.8
	$A^2\Sigma^+$	1.1518	3.56	7.36	13.48	41.7	74.8
	$X^2\Pi$	1.2708	3.06	6.59	7.417	17.9	30.2
$B^{11}N^{14}$	$A^3\Pi$	1.326	1.91	-1.84	6.303	9.07	13.1
	$X^3\Pi$	1.281	3.24	8.13	8.411	21.3	41.7
C_2	$d^1\Sigma_u^+$	1.2378	2.85		11.83	27.2	
	$c^1\Pi_g$	1.2730	2.81		11.57	25.5	
	$b^1\Pi_u$	1.3180	2.76		9.143	19.2	
	$a^1\Sigma_g^+$	1.2422	2.71		12.17	26.6	
	$B^3\Pi_g$	1.5350	4.14		4.328	11.7	
	$A^3\Pi_g$	1.2660	2.56		11.303	22.9	
	$X^3\Pi_u$	1.3117	2.73	4.53	9.523	19.8	25.1
Be^9O^{16}	$B^1\Sigma^+$	1.3622	2.42		6.381	11.3	
	$A^1\Pi$	1.4630	2.66		4.446	8.10	
	$X^1\Sigma^+$	1.3308	2.73	4.53	7.511	15.4	19.4
Be^9F^{19}	$A^2\Pi_i$	1.3942	2.56		4.951	9.11	
	$X^2\Sigma^+$	1.3614	2.61	4.40	5.768	11.0	13.7
F_2^{19}	$B^1\Pi$	1.282	3.28	7.47	7.270	18.6	33.0
	$X^1\Sigma_g^+$	1.412	3.82	8.08	4.726	12.8	19.2
LiF	$X^1\Sigma^+$	1.545	2.57	4.42	2.479	4.12	4.59
B_2^{11}	$A^3\Sigma_u^-$	1.625	2.28		2.850	3.99	
	$X^3\Sigma_g^-$	1.589	2.67	3.74	3.584	6.02	5.31

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
Li_2^7	$B^1\Pi_u$	2.9364	2.16		0.1503	0.111	
	$A^1\Sigma_u^+$	3.1077	1.93		0.1349	0.0838	
	$X^1\Sigma_g^+$	2.6725	1.91	2.00	0.2552	0.182	0.0714
			1-2				
$P^{31}O^{16}$	Σ	1.420	4.10		13.20	38.	
	B	1.434	4.06	8.50	8.451	23.9	34.9
	$A^2\Sigma^+$	1.403	2.97	4.74	12.597	26.7	30.3
	$X^2\Pi$	1.447	2.94	5.13	9.440	19.2	23.1
$P^{31}N^{14}$	$A^1\Pi$	1.5466	3.28		6.913	14.7	
	$X^1\Sigma^+$	1.4910	3.01	5.39	10.52	20.5	24.6
$S^{32}O^{16}$	$B^3\Sigma^-$	1.775	3.58		2.483	5.00	
	$X^3\Sigma^-$	1.4933	3.09	6.22	7.931	16.4	22.1
$N^{14}S^{32}$	$X^2\Pi$	1.4957	2.05		8.318	11.4	
$(Si^{28}O^{16})^+$	$A^2\Sigma$	1.5114	4.60		3.943	12.0	
	$X^2\Sigma$	1.5042	4.52		4.342	13.0	
$Si^{28}O^{16}$	$A^1\Pi$	1.620	3.48	8.33	4.359	9.36	13.8
	$X^1\Sigma$	1.509	2.99	5.73	9.240	18.3	23.2
$C^{12}S^{32}$	$A^1\Pi$	1.5732	3.49		5.910	13.1	
	$X^1\Sigma^+$	1.5344	2.99	5.86	8.489	16.5	21.1
$Cl^{35}O^{16}$	$^2\Pi$	1.54	3.42	6.94	4.892	10.9	14.3
$Si^{28}F^{19}$	?	1.549	1.87	-1.27	6.739	8.13	-3.57
$C^{12}P^{31}$	$B^2\Sigma^+$	1.6892	2.88		3.538	6.03	
	$A^2\Pi_i$	1.671	3.80		5.747	13.1	
	$X^2\Sigma^+$	1.5621	2.93	5.03	7.831	14.6	16.2
$Si^{28}N^{14}$	$B^2\Sigma^+$	1.5800	4.40		5.844	16.3	
	$X^2\Sigma^+$	1.5718	3.04	5.54	7.292	14.1	16.4
$B^{11}S^{32}$	$A^2\Pi$	1.8177	2.90	5.60	2.705	4.32	4.58
	$X^2\Sigma$	1.6071	2.88	5.10	6.720	12.0	13.2

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$Al^{27}O^{16}$	$A^2\Sigma^+$	1.6668	2.78	5.75	4.478	7.46	9.27
	$X^2\Sigma^+$	1.6176	3.30	6.38	5.673	11.6	13.8
$Cl^{35}F^{19}$	$A^3\Pi_o$	1.91	6.29		0.713	2.35	
	$X^1\Sigma$	1.62811	3.14	4.29	4.484	8.65	7.26
$Al^{27}F^{19}$	$B^1\Sigma^+$	1.6170	3.03	2.92	4.932	9.25	5.51
	$A^1\Pi$	1.649	3.24	5.48	4.253	8.34	8.57
	$X^1\Sigma^+$	1.6547	3.12	6.47	4.224	7.95	9.98
$B^{11}Cl^{35}$	$A^1\Pi$	1.6893	3.33		3.351		
	$X^1\Sigma$	1.7157	2.93	5.77	3.4733	5.94	6.81
$Mg^{24}O^{16}$	$B^1\Sigma$	1.737	2.82	4.51	3.839	8.45	5.74
	$A^1\Pi$	1.864	2.99	6.05	2.496	4.01	4.35
	$X^1\Sigma^+$	1.749	2.98	5.11	3.484	5.94	7.50
$Mg^{24}F^{19}$	$X^2\Sigma^+$	1.750	2.80	4.80	3.211	5.13	5.04
			1-3				
$V^{51}O^{16}$	$(A^2\Delta)$	1.672	3.06	2.81	5.377	9.84	5.41
	$(X^2\Delta)$	1.589	2.90	4.53	7.338	14.4	13.2
$Ti^{48}O^{16}$	$C^3\Pi_r$	1.695	2.69		4.960	7.88	
	$X^3\Pi_r$	1.620	2.82	4.18	7.185	12.5	11.4
$Ge^{74}O^{16}$	$A^1\Sigma^+$	1.7861					
	$X^1\Sigma^+$	1.6507	3.15	6.33	7.527	14.4	17.51
$C^{12}Se^{80}$	$X^1\Sigma^+$	1.669	2.90	4.90	6.596	11.5	11.6
$Cu^{63}F^{19}$	$B^1\Sigma$	1.761	4.95		3.715	10.4	
	X	1.743	4.33	16.5	3.333	8.28	18.1
$Br^{79}F^{19}$	$X^1\Sigma^+$	1.75555	5.58		4.072	12.9	
$Ga^{69}F^{19}$	$C^1\Pi$	1.778	4.77	10.7	2.581	6.83	8.72
	$B^3\Pi$	1.7453	3.41	12.0	3.846	7.52	15.1
	$A^3\Pi_{0^+}$	1.7476	3.43	10.8	3.857	7.57	13.6
	$X^1\Sigma^+$	1.7754	3.27	7.4	3.397	6.25	7.99

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$Ca^{40}O^{16}$	$C^1\Sigma$	1.989	3.14	5.25	2.117	3.35	2.81
	$B^1\Pi$	1.950	1.35		2.264	1.57	
	$A^1\Sigma$	1.906	2.02	3.19	3.450	3.65	3.03
	$X^1\Sigma$	1.822	3.07	4.56	3.607	6.08	4.95
$B^{11}Br^{79}$	$A^1\Pi$	1.866	4.81		2.314	5.98	
	$X^1\Sigma^+$	1.887	2.67	4.09	2.665	3.78	3.09
LiBr	$X^1\Sigma^+$	2.1704	2.73	4.23	1.261	1.59	1.13
			1-4				
NbO^{16}	$A^2\Delta$	1.757	2.68	3.38	5.815	8.88	6.36
	$X^2\Delta$	1.691	2.85	4.27	7.863	13.3	11.7
ZrO^{16}	$C^3\Delta$	1.775	2.86	4.6	5.387	8.7	7.9
	$A^3\Phi$	1.752	2.84	4.5	5.875	9.5	8.7
	$X^3\Delta$	1.728	4.26	17.3	7.027	17.3	46.6
SnO^{16}	$D^1\Sigma^+$	1.9628	5.79		2.819	8.07	
	$A^1\Pi$	1.950	3.44	8.29	2.793	4.93	6.09
	$X^1\Sigma^+$	1.832	3.49	8.20	5.612	10.7	13.7
IO	$A^2\Pi_{\frac{3}{2}}$	2.0723	4.06	7.35	2.216	4.35	3.80
	$X^2\Pi_{\frac{3}{2}}$	1.8676	3.65	8.20	3.886	7.58	9.13
SrO^{16}	$^1\Pi$	2.060	2.31		2.155	2.41	
	$C^1\Sigma$	2.132	3.24	6.76	1.837	2.79	2.73
	$A^1\Sigma$	2.027	2.24	4.33	3.053	3.38	3.22
	$X^1\Sigma$	1.923	2.95	3.04	3.403	5.22	2.82
$In^{115}F^{19}$	$C^1\Pi$	1.970	6.45	23.6	2.067	6.76	12.6
	$B^3\Pi_1$	1.9438	3.60	9.76	3.145	5.82	8.12
	$A^3\Pi_{0^+}$	1.9448	3.59	7.15	3.178	5.87	6.01
	$X^1\Sigma^+$	1.9847	3.41	7.83	2.753	4.73	5.47
$Ag^{107}O^{16}$	$X^2\Pi_{\frac{3}{2}}$	1.998	3.26	6.94	1.975	3.23	3.44
	$X^2\Pi_{\frac{1}{2}}$	2.003	3.24	6.27	1.972	3.19	3.13
LiI	$X^1\Sigma^+$	2.3919	2.74	4.34	0.983	1.13	0.745

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
			1-5				
PbO^{16}	$X^1\Sigma^+$	1.922	3.42	6.60	4.557	8.11	8.14
BaO^{16}	$(^1\Sigma?)$	2.2847	2.99	2.63	1.712	2.24	0.863
	$A^1\Sigma$	2.133	2.39	2.98	2.110	2.36	1.38
	$(X)^1\Sigma$	1.940	2.49	3.34	3.787	4.85	3.36
$Tl^{205}F^{19}$	$X^1\Sigma^+$	2.0844	3.39	8.67	2.311	3.75	4.61
CsF^{19}	$X^1\Sigma^+$	2.3453	3.09	7.46	1.452	1.91	1.97
			2-2				
S_2^{32}	$B^3\Sigma_u^-$	2.180	3.64		1.719	2.87	
	$X^3\Sigma_g^-$	1.889	3.21	6.48	4.960	8.44	9.01
	$A^3\Pi^*$	2.28	8.69	75.3	3.373	12.7	48.8
$(Cl_2^{35})^+$	$A^2\Pi$	2.30	5.78	26.7	3.286	8.26	16.6
	$X^2\Pi$	1.891	3.66	9.6	4.289	8.30	11.5
P_2^{31}	$B^1\Sigma_u^+$	2.122	3.24	5.84	2.061	3.14	2.67
	$A^1\Sigma_u^+$	2.1221	3.24				
	$A^1\Pi_g$	1.9883	3.30	6.43	3.495	5.80	5.68
	$X^1\Sigma_g^+$	1.8943	3.01	5.15	5.556	8.82	7.98
	$X^1\Sigma_g$	1.8931	3.09	5.71	5.564	9.07	8.86
$(P_2^{31})^+$	$^2\Pi$	1.9902	3.66		1.735	3.19	3.90
	$^2\Pi$	2.248	3.50		4.053	6.31	7.17
	$X^2\Sigma_g^+$	1.896	3.80		4.909	9.86	
$Si^{28}S^{32}$	$^3\Sigma^-$	2.258	5.01	26.0	1.458		
	$^1\Pi_{ou}$ $^1\Delta$	2.2313	4.99	19.4	1.701	3.80	6.64
	$^1\Sigma^-$	2.301	3.67	13.1	1.441		
	$D^1\Pi$	2.0589	3.60	8.88	2.314		
	$X^1\Sigma^+$	1.9288	3.02	5.73	4.940	7.73	7.61
Cl_2^{35}	$A^3\Pi_{ou}^+$	2.47	5.8		0.590	1.38	
	$X^1\Sigma_g^+$	1.998	3.69	6.1	3.287	6.09	5.1

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
$Al^{27}Cl^{35}$	$a^3\Pi$	2.1041	3.80	5.75	2.467	4.45	6.80
	$A^1\Pi$	2.067	7.7	63.	2.211	8.2	2.6
	$X^1\Sigma^+$	2.138	3.7	12.	2.078	3.6	5.5
Si_2^{28}	$H^3\Sigma_u^-$	2.663	3.11	4.32	0.608	0.712	0.371
	$D^3\Pi_g$	2.155	3.10	5.77	2.48	3.57	3.09
	$X^3\Sigma_g^-$	2.252	3.02	5.87	2.12	2.85	2.46
$Na^{23}Cl$	$X^1\Sigma^+$	2.3606	3.07	5.48	1.101	1.43	1.08
Na_2^{23}	$B^1\Pi_u$	3.4130	2.22		0.1038	0.0676	
	$A^1\Sigma_u^+$	3.639	1.86		0.0936	0.0481	
	$X^1\Sigma_g^+$	3.0986	1.88	1.27	0.1717	0.105	0.023
			2-3				
$Br^{79}Cl^{35}$	$X^1\Sigma^+$	2.138	3.39		2.640	4.18	
$Ga^{69}Cl^{35}$	$X^1\Sigma^+$	2.2017	3.102	7.13	1.821	2.57	2.68
$Al^{27}Br^{79}$	$a^3\Pi$	2.2610	3.54	8.57	1.994	3.12	3.34
	$A^1\Pi$	2.322	5.42		1.046	2.44	
	$X^1\Sigma^+$	2.295	3.12	11.8	1.693	2.30	3.80
CaCl	$C^2\Pi$	2.5160	3.05	5.12	1.242	1.51	1.01
	$X^2\Sigma^+$	2.4390	3.10	6.26	1.504	1.91	1.59
NaBr	$X^1\Sigma^+$	2.5020	3.12	5.45	0.960	1.20	0.836
KCl	$X^1\Sigma^+$	2.6666	3.24	6.37	0.865	1.05	0.775
			2-4				
$I^{127}Cl^{35}$	$B^3\Pi_o^+$	2.61	15.4		0.946	5.62	
	$A^3\Pi_1$	2.7072	2.90		0.710	0.761	
	$X^1\Sigma^+$	2.32070	3.63	7.95	2.384	3.73	5.51
$In^{115}Cl^{35}$	$X^1\Sigma^+$	2.4011	3.28	7.25	1.591	2.17	2.00
$Na^{23}I^{127}$	$X^1\Sigma^+$	2.7115	3.01	5.22	0.763	0.925	0.542
RbCl	$X^1\Sigma^+$	2.7868	3.24	6.16	0.768	0.894	0.609

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
			2-5				
$Ta^{73}O^{16}$	$c^2\Delta$	1.743	3.01	4.0	7.059	12.2	9.3
	$b^2\Pi$	1.744	3.08	4.0	6.977	12.0	9.2
	$(X)a^2\Delta$	1.687	3.22	4.8	9.215	17.0	12.6
$Tl^{205}Cl^{35}$	$X^1\Sigma^+$	2.4848	3.38	5.21	1.454	1.98	1.23
$Cs^{133}Cl$	$X^1\Sigma^+$	2.9062	3.26	6.32	0.720	0.807	0.539
			3-3				
Se_2^{80}	$B^1\Sigma_u^+$	2.45	2.90		1.860	2.20	
	$X^1\Sigma_g^+$	2.157	3.14	4.56	3.613	5.29	3.56
$Br^{79}Br^{81}$	$B^3\Pi_{ou}^+$	2.663	5.99		0.678	1.53	
	$X^1\Sigma_g^+$	2.2836	3.26	4.49	2.458	3.51	2.12
$Ga^{69}Br^{79}$	$X^1\Sigma^+$	2.3525	3.08	5.31	1.499	1.96	1.44
KBr	$X^1\Sigma^+$	2.8207	3.18	6.07	0.707	0.790	0.892
K_2^{39}	$B^1\Pi_u$	4.235	2.26		0.0646	0.0345	
	$X^1\Sigma_g^+$	3.923	2.07	1.16	0.0985	0.0520	0.741
			3-4				
$In^{115}Br^{79}$	$X^1\Sigma^+$	2.5432	3.26	5.49	1.135	1.45	0.964
$Ga^{69}I^{127}$	$X^1\Sigma^+$	2.5747	3.10	6.19	1.232	1.49	1.15
RbBr	$X^1\Sigma^+$	2.9448	3.28		0.670	0.747	
$K^{39}I^{127}$	$X^1\Sigma^+$	3.0478	3.09		0.527	0.534	
			3-5				
$Tl^{205}Br^{79}$		2.6181	3.35	8.02	1.239	1.59	1.45
CsBr		3.0720	3.22		0.568	0.595	
			4-4				
I_2^{127}	$B^3\Pi_{ou}^+$	3.016	5.25		0.612	1.07	
	$X^1\Sigma_g^+$	2.6666	4.00	9.06	1.721	2.58	2.19
$In^{115}I^{127}$	$X^1\Sigma^+$	2.7539	3.26	6.05	1.114	1.32	0.889

	State	r_e	$-a_1$	a_2	F_2	$-F_3$	F_4
RbI	$X^1\Sigma$	3.1769	3.17		0.493	0.492	
			4-5				
$Tl^{205}I^{127}$		2.8135	3.24	10.9	1.04	1.20	1.43
CsI		3.315	3.05		0.396	0.365	

Table III. Parameters for Empirical Functions Relating Force Constants to Bond Length[a]

i	j	a_{ij} F_2	a_{ij} $-F_3$	a_{ij} F_4	b_{ij} F_2	b_{ij} $-F_3$	b_{ij} F_4
H	1	1.54	1.58	1.57	0.64	0.48	0.43
H	2	1.80	1.85	1.77	0.69	0.59	0.47
H	3	1.98	2.01	1.89	0.95	0.74	0.54
H	4	2.08	2.07	2.04	0.96	0.74	0.59
H	5	2.09	2.12	2.04	1.06	0.90	0.69
1	1	1.73	1.78	1.81	0.47	0.39	0.36
1	2	2.02	2.10	2.06	0.53	0.48	0.41
1	3	2.15	2.26	2.08	0.60	0.55	0.34
1	4	2.36	2.41	2.18	0.76	0.57	0.32
1	5	2.47	2.48	2.54	0.87	0.68	0.68
2	2	2.40	2.48	2.35	0.70	0.61	0.46
2	3	2.54	2.57	2.53	0.98	0.72	0.70
2	4	2.63	2.70	2.64	0.96	0.73	0.51
2	5	2.71	2.81	2.60	1.09	1.09	1.30
3	3	2.70	2.77	2.66	1.12	0.89	1.06
3	4	2.66	2.76		1.46	1.19	
3	5	2.73	2.83		1.31	1.05	
4	4	2.85	2.95		0.94	0.70	
4	5	2.84	2.93		1.09	0.78	
H	3T	1.82	1.92		1.04	0.86	
H	4T	1.83			0.75		
H	5T	1.77			0.47		
1	3T	1.98			0.44		
1	4T	2.15			0.52		

[a]Defined by: $r_e = a_{ij} - b_{ij} \log_{10} [(-1)^n F_n]$ for n = 2,3,4.

Average Percentage Deviations from Empirical Relations.[a]

i	j	F_2	F_3	F_4
H	1	4%	4%	7%
H	2	5	6	5
H	3	6	3	6
H	4	3	12	9
H	5	10	5	15
1	1	7	7	9
1	2	6	8	6
1	3	11	11	15
1	4	10	8	20
1	5	10	13	2
2	2	6	3	10
2	3	10	12	20
2	4	10	13	25
2	5	10	2	5
3	3	12	7	15
3	4	5	6	
3	5	3	2	
4	4	10	3	
4	5	2	15	
H	3T	4	2	
H	4T	4		
H	5T	9		
1	3T	6		
1	4T	5		

[a] The tabulated quantity is the average of $100 \times |(F_n)_{calc} - (F_n)_{obs}|/|F_n|_{obs}$ for each family of molecules.

Some Cases Showing Especially Large Deviations.[a]

Molecule	F_2	F_3	F_4
$(OH)^+$	23%	30%	9%
LiH	-20	-23	- 9
LiD	-15	-24	-12
$(HCl)^+$	22	5	18
$(DCl)^+$	30	14	
$(AlH)^+$	31	15	
InH	23	22	43
TlH	38	27	23
BF	21	22	45
F_2	-0 4	-31	-33
B_2	- 44	-49	-23
Li_2	- 96	-75	-43
SO	25	12	10
NS	17	60	
$(SiO)^+$	117	33	
ClF	23	11	55
BrF	12	-36	
LiBr	-27	- 7	-52
GaF	21	22	- 2
BaO	7	29	126
Cl_2^+	19	3	-14
Si_2	-23	-17	-33
Na_2	-42	- 3	- 1
GaCl	21	26	10
GaBr	36	50	35

[a] The percentage deviation is listed for the ground electronic state.

Table IV. Cubic Force Constants for Bond Stretching in Polyatomic Molecules

Bond	Molecule	Bond Length	$-F_3$, Cubic Constant Expt.	Predicted
CH	CH_4	1.09	10	10
	HCN	1.06	12	12
	DCN	1.06	11	12
	HCCH	1.06	11	12
	DCCD	1.06	11	12
CC	HCCH	1.20	32	30
	DCCD	1.20	33	30
CN	HCN	1.16	44	39
	DCN	1.16	42	39
CO	CO_2	1.16	38.5	39
	OCS	1.16	36	39
CS	CS_2	1.55	14	14
	OCS	1.55	16	14
CSe	OCSe	1.71	10	10
CBr	BrCN	1.79	6.8	7.2
CI	ICN	1.99	4.9	5.5
OH	H_2O	0.96	19.8	19.5
NO	$N_2^{14}O$	1.19	33	33
	$N^{15}N^{14}O$	1.19	33	33
NN	$N_2^{14}O$	1.13	39	46
	$N^{15}N^{14}O$	1.13	44	46

Bibliography for Table IV

Molecule	Reference for Spectroscopic Data
CH_4	K. T. Hecht, J. Mol. Spect. 5, 390 (1960). L. H. Jones and R. S. McDowell, ibid., 3, 632 (1959).
HCN DCN	D. H. Rank, G. Skorinko, D. P. Eastman, and T. A. Wiggins, J. Opt. Soc. Am. 50, 421 (1960).
HCCH	J. Overend, Trans. Faraday Soc. 56, 310 (1960), and references cited therein.
CO_2	C. P. Courtoy, Can J. Phys. 35, 608 (1957).
CS_2	A. H. Guenther, J. Chem. Phys. 31, 1095 (1959).
OCS OCSe ICN BrCN	C. H. Townes and A. L. Schawlow, Microwave Spectroscopy (McGraw Hill, New York, 1955).
H_2O	Benedict, Gailar, and Plyler, J. Chem. Phys. 24, 1139 (1956).
N_2O	A. E. Douglas and C. K. Møller, J. Chem. Phys. 22, 275 (1954).