Title
BIBLIOGRAPHY FOR HINDERED INTERNAL ROTATION AND MICROWAVE SPECTROSCOPY

Author
Herschbach, D.R.

Publication Date
1962-10-01

UCRL-10404

University of California

Ernest O. Lawrence Radiation Laboratory

BIBLIOGRAPHY FOR HINDERED INTERNAL ROTATION AND MICROWAVE SPECTROSCOPY

Berkeley, California

DISCLAIMER

UCRL-10404
UC-4 Chemistry
TID-4500 (18th Ed.)

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

BIBLIOGRAPHY FOR HINDERED INTERNAL ROTATION AND MICROWAVE SPECTROSCOPY

D. R. Herschbach

October 1962

Printed in USA. Price 75 cents. Available from the
Office of Technical Services
U. S. Department of Commerce
Washington 25, D.C.

BIBLIOGRAPHY FOR HINDERED INTERNAL ROTATION AND MICROWAVE SPECTROSCOPY

D. R. Herschbach
Department of Chemistry and Lawrence Radiation Laboratory,
University of California, Berkeley, California

This report has been prepared to supplement a review of microwave studies of internal rotation given in UCRL-10405. Several tables summarizing experimental results are provided, together with an extensive bibliography.

The molecules studied and molecular parameters derived from the spectra are listed in Table I. This is intended to include all microwave studies published up to September, 1962. In a few cases results obtained from thermodynamic measurements or infrared spectroscopy are included (as indicated by a superscript c or d), when these supplement the microwave data. Results derived from microwave intensity measurements rather than frequency measurements are also specifically indicated (by a superscript e). When several literature references are given, the one which is regarded as providing the best value of the barrier height is underlined, and the one which provides the best structural parameters is indicated by an asterisk.

A more compact list of the barrier values is given in Tables II-IV. The barriers listed in Tables I and II for internal rotation of CH_3 and SiH_3 groups refer to a hindering potential of the form

$$V(\alpha) = \tfrac{1}{2}V_N(1-\cos N\alpha) + \tfrac{1}{2}V_{2N}(1-\cos 2N\alpha) + \ldots, \qquad (1)$$

where α is the angle of internal rotation about the symmetry axis of the group and the periodicity N=3, except for CH_3BF_2 and CH_3NO_2 for which N=6. The tabulated barrier heights are nominally values of V_N, as only the leading term in (1) has been retained in analyzing the data. In a few cases, listed in Table III, an estimate of the V_{2N} coefficient has been obtained. However, since this introduces only a small correction to the barrier shape, the contribution of V_{2N} and higher terms in (1) cannot be disentangled from other small perturbations (such as vibrational interactions) which are not included in the analysis. The values of V_{2N} in Table III thus only represent approximate upper limits. The uncertainty in the V_N values of Table II is usually about ±5%. This arises mainly from the uncertainty in the structural parameters (especially the moment of inertia I_α of the CH_3 or SiH_3 groups) that enter the analysis. The structural uncertainties are in turn due primarily to the lack of a feasible way to correct for vibration-rotation perturbations. In Table IV are listed the few examples studied so far of barriers having less than threefold periodicity. The potential function assumed and probable uncertainty in the derived values of the coefficients is indicated for each case.

Table V lists several molecules for which the equilibrium configuration of the internal rotor group has been established.

Table VI collects examples for which the "angle of tilt" between the bond direction and the symmetry axis of an internal rotor group has been determined.

The remaining tables provide a convenient index to theoretical papers on internal rotation. Table VII consists of references which deal with energy level calculations and the analysis of microwave spectra, Table VIII lists the available tabulations of Mathieu eigenvalues and related functions, and Table IX gives references concerned with the origin of the potential barriers.

The bibliography includes and extends that provided by C. C. Lin and J. D. Swalen, Rev. Mod. Phys. 31, 841 (1959). The references are arranged by year and within each year alphabetically according to the name of the first author. If a paper is not directly concerned with microwave spectroscopy the reference number is underlined.

The author is greatly indebted to Miss Nancy Monroe for her aid in compiling the bibliography.

Table I. Microwave studies of internal rotation.

Formula	Compound	V_3[a]	Other Data[a]	References[b]
		C-C Bonds		
CH_3CH_3	ethane	2.9[c,d]	I	31,123,131*
CH_3CH_2F	ethyl fluoride	3.31	I,ETS	64,80,132,152*
CH_3CHF_2	1,1-difluoroethane	3.18	ETS	53,80
CH_3CF_3	methyl fluoroform	3.5[e]	I,ETS	19,29
CH_2FCF_3	1,1,1,2-tetrafluoroethane	4.2[d]		133
CH_3CH_2Cl	ethyl chloride	3.69	I,ETS	55,74,115,142,191*
CH_3CH_2Br	ethyl bromide	3.57	I,ETS	75,116,142
CH_3CH_2I	ethyl iodide	2.4[f]		137a
CH_3CH_2CN	ethyl cyanide	3.05	ETS,EVS	105,141
$CH_3CH_2CH_3$	propane	>2.7	I	162
$CH_3CH_2SiH_3$	ethyl silane	2.65	I,ETS	198
c-CH_3CH_2CHO	cis-propionaldehyde	2.7		193,195
$CH_3CH_2CH_2F$	propyl fluoride trans isomer gauche isomer	 2.69 2.87	 ETS EVS	184
$(CH_3)_3CH$	isobutane	3.9[e]	I,ETS,EVS	125,163*
$(CH_3)_3CF$	t-butyl fluoride	4.3[e]	ETS	125
CH_3CHO	acetaldehyde	1.17	I	85,98*,132,136
CH_3COF	acetyl fluoride	1.04	I	146
CH_3COCl	acetyl chloride	1.30	I	180
CH_3COBr	acetyl bromide	1.30	I	158
CH_3COCN	acetyl cyanide	1.27	I	138,157
CH_3COOH	acetic acid	0.48	I	114

Formula	Compound	V_3[a]	Other Data[a]	References[b]
$(CH_3)_2CO$	acetone	0.76	I	149
$CH_3COC_2H_5$	cis-butanone	0.50	I	200
$CH_3CH=CH_2$	propylene	1.98	I	107,121,175*
t-$CH_3CH=CHF$	trans 1-fluoro-propene	2.15		111
c-$CH_3CH=CHF$	cis 1-fluoro-propene	1.06		182
$CH_3CF=CH_2$	2-fluoro-propene	2.44	ETS	147
t-$CH_3CH=CHCN$	trans-crotono-nitrile	>2.1		161
$CH_3CH=C=O$	methyl ketene	1.20		181
$CH_3CH=C=CH_2$	methyl allene	1.59		108
$(CH_3)_2C=CH_2$	isobutylene	2.21	I	173
$CH_3\overset{O}{\diagdown\diagup}CH-CH_2$	propylene oxide	2.56	ETS	112,122
c-$CH_3\overset{O}{\diagdown\diagup}CH-CHCH_3$	cis 2,3-epoxy-butane	1.61		179
$CH_3C\equiv CCH_2Cl$	1-chloro-butyne-2	<0.050		141
$CH_3C\equiv CCF_3$	1-trifluoro-butyne-2	<0.3	I	37,65,90

Other C-IV Bonds

CH_3SiH_3	methyl silane	1.66	I,ETS,NR	23,47,99* 136
CH_3SiH_2F	methyl fluoro-silane	1.56	I	128,156
CH_3SiHF_2	methyl difluoro-silane	1.26	I	131,156
CH_3SiF_3	methyl tri-fluorosilane	1.2[b]	I,ETS,EVS	24,29,32

Formula	Compound	V_3[a]	Other Data[a]	References[b]
$(CH_3)_2SiH_2$	dimethyl silane	1.67	I,ETS	145,177
$(CH_3)_3SiH$	trimethyl silane	1.8[e]	I,ETS	165
$SiH_3C_2H_5$	ethyl silane	1.98	I,ETS	198
SiH_3CH_2Cl	chloromethyl silane	2.55	I,ETS	192
$SiH_3CH_2{=}CH_2$	vinyl silane	1.50	I,ETS	176
CH_3GeH_3	methyl germane	1.24	I,ETS	118,139*
CH_3SnH_3	methyl stannane	0.65	I,ETS,NR	167
		C-V Bonds		
CH_3NH_2	methyl amine	1.98	I,ETS,NR	16,35,40,43,44,48,51,52,68,81,102,106*,110
$(CH_3)_2NH$	dimethyl amine	3.4[d]		183,197
$(CH_3)_2N$	trimethyl amine	4.4[e]	ETS	124,183
CH_3PH_2	methyl phosphine	1.96		172
$(CH_3)_2PH$	dimethyl phosphine	2.20		200
$(CH_3)_3P$	trimethyl phosphine	2.6[e]	ETS	125
CH_3AsF_2	methyl difluoroarsine	1.33		189
$(CH_3)_3As$	trimethyl arsine	1.5-2.5[e]		142a
		C-VI Bonds		
CH_3OH	methyl alcohol	1.07	I,ETS,NR	15,16,17,26,27,39,70,72,73*,87,94,113
CH_3OCl	methyl hypochlorite	>3		201
CH_3OOCH	methyl formate	1.19	I	132a

Formula	Compound	V_3[a]	Other Data[a]	References[b]
CH_3ONO_2	methyl nitrate	2.32	ETS,EVS	168
$(CH_3)_2O$	dimethyl ether	2.72		137
$t\text{-}CH_3OC_2H_5$	ethyl methyl ether	2.53	I,ETS	199
CH_3SH	methyl mercaptan	1.27	I,ETS,NR	60,63,69, 103,160
$(CH_3)_2S$	dimethyl sulfide	2.10	I,ETS	166,178*, 190
		Sixfold Barriers		
		V_6 (cal/mole)		
CH_3BF_2	methyl boron difluoride	13.77		109
CH_3NO_2	nitromethane	6.03	I	58,89

Molecules with one- or twofold barriers are listed in Table IV.

[a] Values of barrier heights are given in kcal/mole; to convert to cm^{-1} units, multiply by 0.3498. An I indicates that two or more isotopic species have been studied; ETS or EVS that the rotational spectra of excited torsional or vibrational states have been analyzed; NR that the parameters for a "nonrigid" model have been evaluated (see Table VII, under "interaction of vibration-internal rotation-overall rotation"). Other tables collect references to information about corrections to the barrier shape (Table III) and equilibrium configurations (Tables V and VI).

[b] See the bibliography. When several references are given, the one which gives the best value of the barrier height is underlined, and the one which gives the best structural parameters is indicated by an asterisk.

[c]From thermodynamic measurements.

[d]From infrared spectroscopy.

[e]From microwave intensity measurements.

[f]The reported value is probably quite inaccurate.

Table II. Barrier heights (kcal/mole).

C-C Bonds

CH_3CH_3	2.9[a]	CH_3CHO	1.17	$CH_3CH=CH_2$	1.98
CH_3CH_2F	3.31	CH_3COF	1.04	t-$CH_3CH=CHF$	2.15
CH_3CHF_2	3.18	CH_3COCl	1.30	t-$CH_3CH=CHCl$	2.17
CH_3CF_3	3.5[b]	CH_3COBr	1.30	c-$CH_3CH=CHF$	1.06
CH_3CH_2Cl	3.56	CH_3COCN	1.27	$CH_3CF=CH_2$	2.44
CH_3CH_2Br	3.57	CH_3COOH	0.48	t-$CH_3CH=CHCN$	>2.1
CH_3CH_2CN	3.05	$(CH_3)_2CO$	0.76	$CH_3CH=C=O$	1.20
$CH_3CH_2CH_3$	>2.7	$CH_3COC_2H_5$	0.50	$CH_3CH=C=CH_2$	1.59
$CH_3CH_2SiH_3$	2.65			$(CH_3)_2C=CH_2$	2.21
c-CH_3CH_2CHO	2.7			$CH_3CH\text{-}CH_2$ (O)	2.56
t-$CH_3CH_2CH_2F$	2.69			c-$CH_3CH\text{-}CHCH_3$ (O)	1.61
g-$CH_3CH_2CH_2F$	2.87				
$(CH_3)_3CH$	3.9[b]			$CH_3C\equiv CCH_2Cl$	<0.050
$(CH_3)_3CF$	4.3[b]				

Other C-IV Bonds

CH_3SiH_3	1.66
CH_3SiH_2F	1.56
CH_3SiHF_2	1.26
CH_3SiF_3	1.2[b]
$(CH_3)_2SiH_2$	1.67
$(CH_3)_3SiH$	1.8[b]
$SiH_3C_2H_5$	1.98
SiH_3CH_2Cl	2.55
$SiH_3CH_2{=}CH_2$	1.50
CH_3GeH_3	1.24
CH_3SnH_3	0.65

C-V Bonds

CH_3NH_2	1.98
$(CH_3)_2NH$	3.4[a]
$(CH_3)_3N$	4.4[b]
CH_3PH_2	1.96
$(CH_3)_2PH$	2.20
$(CH_3)_3P$	2.6[b]
CH_3AsF_2	1.33
$(CH_3)_3As$	2[b]

C-VI Bonds

CH_3OH	1.07
CH_3OCl	>3
CH_3OOCH	1.19
CH_3ONO_2	2.32
$(CH_3)_2O$	2.72
t-$CH_3OC_2H_5$	2.53
CH_3SH	1.27
$(CH_3)_2S$	2.10

Sixfold Barriers (cal/mole)

CH_3BF_2	13.77
CH_3NO_2	6.03
CD_3NO_2	5.19

[a]From thermodynamic data or infrared spectra.

[b]From microwave intensity measurements.

Table III. Corrections to barrier shape (kcal/mole).[a]

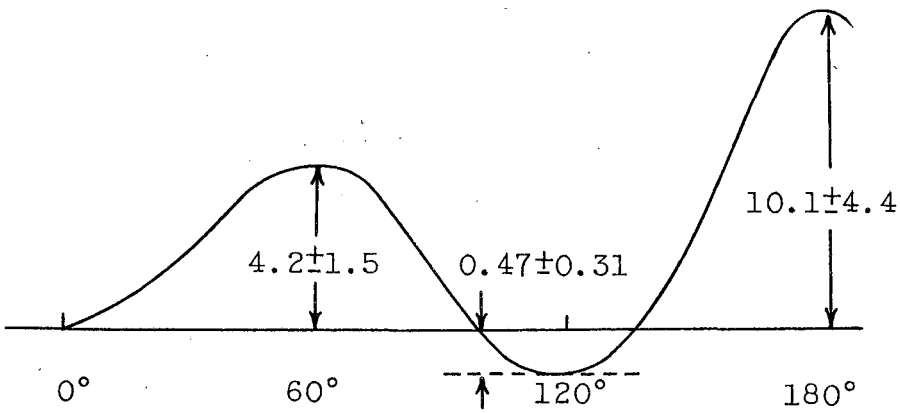
Molecule	V_3	V_6	V_6/V_3	Ref.
CH_3CH_2Cl	3.69±0.30	0±0.003	~0%	196a
	3.69±0.10			191
$CH_3CH=CH_2$	2.03±0.30	-0.045±0.003	-2.3%	196a
	1.98±0.17			107
$CH_3CF=CH_2$	2.34±0.10	0.011±0.003	0.6%	196a
	2.46±0.05	<0.050	<2.5	147
$CH_3CH\text{-}CH_2$ (O)	2.58±0.23	-0.026±0.003	-1.0%	196a
	2.56±0.72	<0.030	<1%	122

[a]The indicated uncertainties refer to the spectral analysis, and do not include an allowance for the idealizations of the molecular model used in interpreting the spectra.

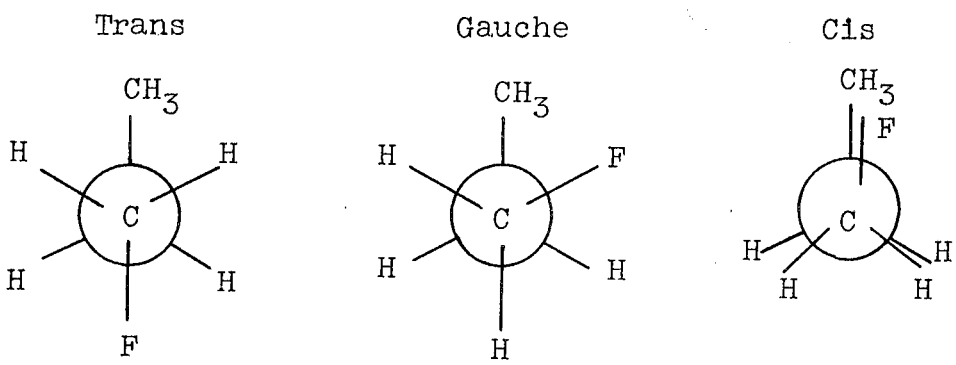
Table IV. Twofold and onefold barriers (kcal/mole).

Formula	Compound	Reference
$CH_3CH_2CH_2F$	n-propyl fluoride	184

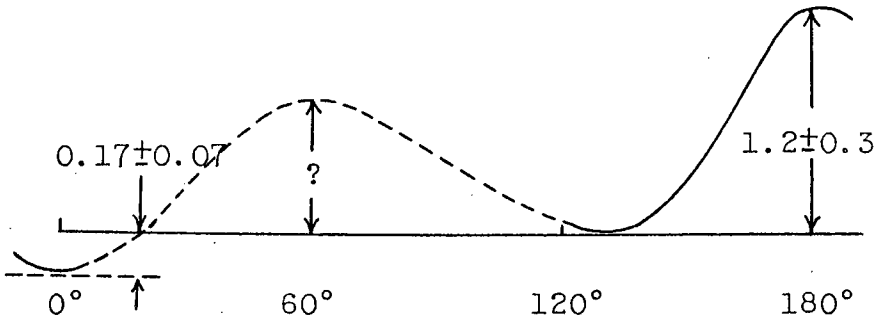
$$V(\alpha) = \Sigma_n \tfrac{1}{2}V_n(1-\cos n\alpha)$$

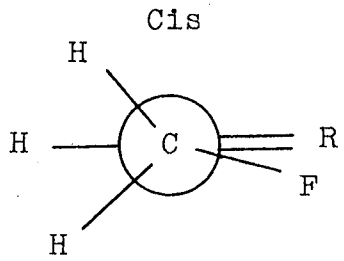


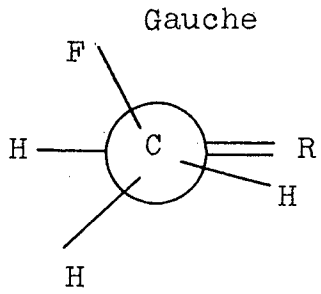
V_1=3.22±2.02
V_2=-3.05±1.72
V_3=6.48±2.15
V_4=-1.25±1.17



Formula	Compound	Reference
$CH_2FCH=CH_2$	allyl fluoride	196







C_6H_5OH phenol 159

$$V(\alpha) = \frac{1}{2}V_2(1-\cos 2\alpha)$$

$V_2 = 3.15\pm0.3$

$\alpha = 0°, 180°$ for planar configuration

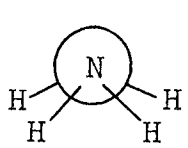
Formula	Compound	Reference
NH_2NH_2	hydrazine	185

$$V(\alpha) = \tfrac{1}{2}V_2(1+\cos 2\alpha)$$

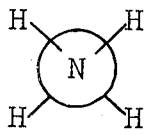
$V_2 = 3.15 \pm 0.15$

$V_2 = V_{cis} = V_{trans}$ assumed

$\alpha \approx 90°$ at potential minimum



Cis (α=0°)



Trans (α=180°)

NF_2NF_2	tetrafluorohydrazine	143

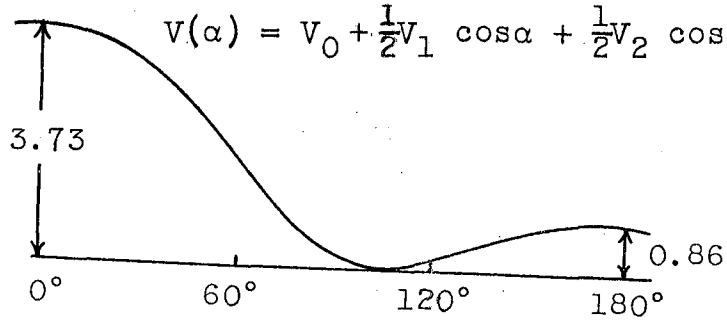
$V_2 > 3$

$\alpha \approx 65°$ at potential minimum

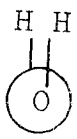
H_2O_2	hydrogen peroxide	50, 86, 163a, 189a

$$V(\alpha) = V_0 + \tfrac{1}{2}V_1 \cos\alpha + \tfrac{1}{2}V_2 \cos 2\alpha$$

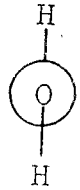
V_0=1.22
V_1=2.86
V_2=2.15



Cis



Trans



α = 109.5° at potential minimum

$\langle\alpha\rangle$ = average dihedral angle

= 119.8°

Table V. Equilibrium configurations.

Compound	Configuration	References
	C-C Bonds	
CH_3CH_2F	Staggered	152
CH_3CH_2Cl	Staggered	74
$CH_3CH_2CH_3$	Both methyl groups staggered with respect to methylene group	162
$(CH_3)_3CH$	Each methyl group staggered with respect to methine group	163
CH_3CHO	Methyl group eclipses O and staggers H	98
CH_3COF	Methyl group eclipses O and staggers F	146
CH_3COCl	Methyl group eclipses O and staggers Cl	180
CH_3COCN	Methyl group eclipses O and staggers CN	138
$CH_3CH=CH_2$	Methyl group eclipses double bond and staggers methine H	121
$(CH_3)_2C=CH_2$	Both methyl groups eclipse double bond	173
	Other C-IV Bonds	
CH_3SiH_3	Staggered	99
CH_3SiH_2F	Staggered	128
CH_3SiHF_2	Staggered	156
$(CH_3)_3SiH$	Each methyl group staggered with respect to siline group	165

Compound	Configuration	References
$SiH_3CH=CH_2$	Silyl group staggered with respect to methine group	176
CH_3GeH_3	Staggered	139
	C-VI Bonds	
CH_3OOCH	Methyl group staggered with respect to formyl group	132a
C_6H_5OH	Planar	159
$(CH_3)_2S$	Both methyl groups staggered with respect to the adjacent CS bond	178
	Other Bonds	
NH_2NH_2	Dihedral angle = 90°	185
NF_2NF_2	Dihedral angle = 65°	143
H_2O_2	Dihedral angle = 120°	189a
	Rotational Isomers	
$CH_3CH_2CH_2F$	Gauche configuration of CH_3 and F slightly more stable than trans	184
$CH_3CH_2CH_2CN$	Gauche configuration of CH_3 and CN slightly more stable than trans	196
$CH_2FCH=CH_2$	Cis configuration of F and $C=CH_2$ group slightly more stable than trans	196

Table VI. Angles of tilt.

Molecule	Bond	θ[a]	Reference
$(CH_3)_2SiH_2$	C-Si	0°	177
CH_3NH_2	C-N	3°	106
CH_3OH	C-O	5°	94
$(CH_3)_2O$	C-O	5°	137
CH_3SH	C-S	2.5°	160
$(CH_3)_2S$	C-S	2.5°	178

[a] θ is the angle between the symmetry axis of the methyl group and the bond about which internal rotation occurs. The uncertainty in the experimental values is about ± 0.5 to $\pm 1°$.

Table VII. Papers treating mechanics of internal rotation.

Partition functions for internal rotation
5,9,14,20,22,59,84,92,120
Energy levels including coupling of internal and over-all rotation
Two coaxial symmetric tops: 2,3a,6,36a
Symmetric top attached to asymmetric frame:
5,9,26,39,63,76,78,81,87,88,89,93, 97,98,103,107,112,122,136
Two symmetric tops attached to asymmetric frame:
5,9,136,137,145,149,164,169,177,179,188,190
Two asymmetric tops:
8,10,14,20,38,50,86,153,185
Interaction of vibration with internal and overall rotation
47,61,62,83,87,94,101,102,106,110,113,140,196b
Reviews
7,12,126,144

Table VIII. Tabulations of Mathieu eigenvalues and integrals.[a]

References	Period in x	Range in v	Range in s
33[b,c]	$\pi, 2\pi$	0(1)8	0(1)100
		9(1)14	0(2)100
56[d]	$\pi, 2\pi$	0(1)15	100-∞
82[c]	3π	0(1)5	2(1)30(2)52(4)100
84	4π	0(1)9	1(1)40
95,96[e,f]	$\pi, 3\pi$	0(1)7	2(2)12(4)100
129	$\pi, 3\pi$	0(1)4	100(15)205
136[e,f]	$\pi, 3\pi$	0(1)2	8(4)100
171,199[e]	$\pi, 2\pi, 3\pi$ $4\pi, 5\pi, 6\pi$	0(1)16	0(2)100(4)200

[a] For notation see, for example, reference 136.

[b] A close tabulation is given for low s values.

[c] Eigenfunctions are also tabulated.

[d] Tabulated in terms of a parameter t=0(0.002)0.1, where $s=1/t^2$.

[e] Perturbation coefficients and matrix elements required for the treatment of coupling of internal and over-all rotation are tabulated.

[f] Relations are given which enable results to be derived for barriers of any periodicity.

Table IX. Papers treating origin of potential barriers.

Quantum mechanical approximations
Numerical results: 1,4,135,155
Semi-empirical or qualitative: 119,127,130,154a
Steric repulsion
11,13,28,36,41,42,49,66,67,77,104,150,186
Electrostatic interaction
8,21,25,30,45,154
Reviews
31,117,151

BIBLIOGRAPHY

1932

1. H. Eyring, J. Am. Chem. Soc. 54, 3191.

2. H. H. Nielsen, Phys. Rev. 40, 445.

1935

3. E. B. Wilson, Jr., J. Chem. Phys 3, 276.

1937

3a. J. B. Howard, J. Chem. Phys. 5, 442, 451.

1939

4. Gorin, Walter, and Eyring, J. Am. Chem. Soc. 61, 1876.

1940

5. B. L. Crawford, J. Chem. Phys. 8, 273.

6. J. S. Koehler and D. M. Dennison, Phys. Rev. 57, 1006.

7. E. B. Wilson, Jr., Chem. Revs. 27, 17.

1941

8. D. Price, J. Chem. Phys. 9, 807.

1942

9. K. S. Pitzer and W. D. Gwinn, J. Chem. Phys. 10, 428.

10. D. Price, J. Chem. Phys. 10, 80.

1944

11. Aston, Isserow, Szasz, and Kennedy, J. Chem. Phys. 12, 336.

1945

12. G. Herzberg, Infrared and Raman Spectra (D. Van Nostrand Company, Inc., Princeton, New Jersey.

1946

13. French and Rasmussen, J. Chem. Phys. 14, 389.

14. K. S. Pitzer, J. Chem. Phys. 14, 239.

1947

15. B. P. Dailey, Phys. Rev. 72, 84.

16. W. D. Herschberger and J. Turkevich, Phys. Rev. 71, 554.

1948

17. D. K. Coles, Phys. Rev. 74, 1194.

18. Lasettre and Dean, J. Chem. Phys. 16, 151.

1949

19. Dailey, Shulman, and Minden, Phys. Rev. 75, 1319A.

20. J. E. Kilpatrick and K. S. Pitzer, J. Chem. Phys. 17, 1064.

21. Lasettre and Dean, J. Chem. Phys. 17, 317.

1950

22. J. O. Halford, J. Chem. Phys. 18, 444.

23. D. R. Lide, Jr. and D. K. Coles, Phys. Rev. 80, 911.

24. Minden, Mays, and Dailey, Phys. Rev. 78, 347A.

1951

25. Au Chin Tang, J. Chinese Chem. Soc. 18, 1.

26. D. G. Burkhard and D. M. Dennison, Phys. Rev. 84, 408.

27. Hughes, Good, and Coles, Phys. Rev. 84, 418.

28. Luft, Discussions Faraday Soc. 10, 117.

29. H. Minden and B. P. Dailey, Phys. Rev. 82, 338A.

30. Oosterhoff, Discussions Faraday Soc. 10, 79.

31. K. S. Pitzer, Discussions Faraday Soc. 10, 66.

32. J. Sheridan and W. Gordy, J. Chem. Phys. 19, 965.

33. Tables Relating to Mathieu Functions (Columbia University Press, New York, 1951).

1952

34. B. P. Dailey, Ann. N. Y. Acad. Sci. 55, 915.

35. D. R. Lide, Jr., J. Chem. Phys. 20, 1812.

36. J. Van Dranen, J. Chem. Phys. 20, 1982.

36a. H. T. Minden, J. Chem. Phys. 20, 1964.

1953

37. Bak, Hansen, and Anderson, J. Chem. Phys. 21, 1612.

38. D. G. Burkhard, J. Chem. Phys. 21, 1541.

39. E. V. Ivash and D. M. Dennison, J. Chem. Phys. 21, 1804.

40. D. R. Lide, Jr., J. Chem. Phys. 21, 571.

41. Luft, J. Chem. Phys. 21, 179.

42. Luft, Trans. Faraday Soc. 49, 118.

43. K. Shimoda and T. Nishikawa, J. Phys. Soc. Japan 8, 133.

44. K. Shimoda and T. Nishikawa, J. Phys. Soc. Japan 8, 425.

1954

45. Au Chin Tang, Sci. Sinica 3, 279.

46. D. H. Baird and G. R. Bird, Rev. Sci. Instr. 25, 319.

47. D. Kivelson, J. Chem. Phys. 22, 1733.

48. D. R. Lide, Jr., J. Chem. Phys. 22, 1613.

49. Luft, J. Chem. Phys. 22, 155, 1814.

50. J. T. Massey and D. R. Bianco, J. Chem. Phys. 22, 442.

51. Shimoda, Nishikawa, and Itoh, J. Phys. Soc. Japan 9, 974.

52. Shimoda, Nishikawa, and Itoh, J. Chem. Phys. 22, 1456.

53. N. Solimene and B. P. Dailey, J. Chem. Phys. 22, 2042.

54. Tannenbaum, Johnson, Myers, and Gwinn, J. Chem. Phys. 22, 949.

55. R. S. Wagner and B. P. Dailey, J. Chem. Phys. 22, 1459.

1955

56. G. Blanch and I. Rhodes, Wash. Acad. Sci. 45, 166.

57. D. G. Burkhard and J. C. Irvin, J. Chem. Phys. 23, 1355.

58. W. D. Gwinn, Faraday Soc. Disc. 19, 43.

59. Ivash, Li, and Pitzer, J. Chem. Phys. 23, 1814.

60. R. W. Kilb, J. Chem. Phys. 23, 1736.

61. D. Kivelson, J. Chem. Phys. 23, 2230.

62. D. Kivelson, J. Chem. Phys. 23, 2236.

63. T. Kojima and T. Nishikawa, J. Phys. Soc. Japan 10, 240.

64. J. Kraitchman and B. P. Dailey, J. Chem. Phys. 23, 184.

65. D. R. Lide, Jr. and D. Kivelson, J. Chem. Phys. 23, 2191.

66. Luft, Z. Elektrochem. 59, 46.

67. E. A. Mason and M. M. Kreevoy, J. Am. Chem. Soc. 77, 5808.

68. Nishikawa, Itoh, and Shimoda, J. Chem. Phys. 23, 1735.

69. N. Solimene and B. P. Dailey, J. Chem. Phys. 23, 124.

70. J. D. Swalen, J. Chem. Phys. 23, 1739.

71. C. H. Townes and A. L. Schawlow, Microwave Spectroscopy (McGraw-Hill Book Company, Inc., New York, 1955).

72. Venkateswarlu, Edwards, and Gordy, J. Chem. Phys. 23, 1195.

73. P. Venkateswarlu and W. Gordy, J. Chem. Phys. 23, 1200.

74. R. S. Wagner and B. P. Dailey, J. Chem. Phys. 23, 1355.

75. Wagner, Solimene, and Dailey, J. Chem. Phys. 23, 599.

76. Wilson, Lin, and Lide, J. Chem. Phys. 23, 136.

1956

77. B. Bak, J. Chem. Phys. 24, 918.

78. D. G. Burkhard, Trans. Faraday Soc. 52, 1.

79. T. Das, J. Chem. Phys. 25, 896.

80. D. R. Herschbach, J. Chem. Phys. 25, 358.

81. T. Itoh, J. Phys. Soc. Japan 11, 264.

82. R. W. Kilb, "Tables of Mathieu Eigenvalues and Eigenfunctions Mathieu for Special Boundary Conditions," Department of Chemistry, Harvard University.

83. D. Kivelson, J. Chem. Phys. 26, 215.

84. J. C. M. Li and K. S. Pitzer, J. Phys. Chem. 60, 466.

85. C. C. Lin and R. W. Kilb, J. Chem. Phys. 24, 631.

86. J. T. Massey and R. W. Hart, J. Chem. Phys. 23, 942.

87. T. Nishikawa, J. Phys. Soc. Japan 11, 781.

88. J. D. Swalen, J. Chem. Phys. 24, 1072.

89. Tannenbaum, Myers, and Gwinn, J. Chem. Phys. 25, 42.

1957

90. Bak, Christensen, Hansen-Nygaard, and Tannenbaum, J. Chem. Phys. 26, 241.

91. T. Das, J. Chem. Phys. 27, 763.

92. J. O. Halford, J. Chem. Phys. 26, 851.

93. K. T. Hecht and D. M. Dennison, J. Chem. Phys. 26, 31.

94. K. T. Hecht and D. M. Dennison, J. Chem. Phys. 26, 48.

95. D. R. Herschbach, "Tables for the Internal Rotation Problem," Department of Chemistry, Harvard University.

96. D. R. Herschbach, J. Chem. Phys. 27, 975.

97. D. R. Herschbach, J. Chem. Phys. 27, 1420.

98. Kilb, Lin, and Wilson, J. Chem. Phys. 26, 1695.

99. R. W. Kilb and L. Pierce, J. Chem. Phys. 27, 108.

101. D. Kivelson, J. Chem. Phys. 27, 980.

102. D. Kivelson and D. R. Lide, Jr., J. Chem. Phys. 27, 353.

103. T. Kojima and T. Nishikawa, J. Phys. Soc. Japan 12, 680.

104. M. M. Kreevoy and E. A. Mason, J. Am. Chem. Soc. 79, 4851.

105. R. G. Lerner and B. P. Dailey, J. Chem. Phys. 26, 678.

106. D. R. Lide, Jr., J. Chem. Phys. 27, 343.

107. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys 27, 868.

108. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys. 27, 874.

109. R. E. Naylor, Jr. and E. B. Wilson, Jr., J. Chem. Phys. 26, 1057.

110. T. Nishikawa, J. Phys. Soc. Japan 12, 668.

111. S. Siegal, J. Chem. Phys. 27, 989.

112. J. D. Swalen and D. R. Herschbach, J. Chem. Phys. 27, 100.

113. P. R. Swan and M. W. P. Strandberg, J. Mol. Spectroscopy 1, 33.

114. W. J. Tabor, J. Chem. Phys. 27, 974.

115. R. S. Wagner and B. P. Dailey, J. Chem. Phys. 26, 1588.

116. Wagner, Dailey and Solimene, J. Chem. Phys. 26, 1593.

117. E. B. Wilson, Jr., Proc. Natl. Acad. Sci. U.S. 43, 816.

1958

118. A. I. Barchukov and A. M. Prokhorov, Optika i Septroskopia 4, 799.

119. Eyring, Stewart, and Smith, Proc. Natl. Acad. Sci. U.S. 44, 259.

120. S. Golden, J. Phys. Chem. 62, 74.

121. D. R. Herschbach and L. C. Krisher, J. Chem. Phys. 28, 728.

122. D. R. Herschbach and J. D. Swalen, J. Chem. Phys. 29, 761.

123. D. R. Lide, Jr., J. Chem. Phys. 29, 1426.

124. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys. 28, 572.

125. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys. 29, 914.

126. C. C. Lin, Amer. J. Phys. 26, 319.

127. L. Pauling, Proc. Natl. Acad. Sci. U.S. 44, 211.

128. L. Pierce, J. Chem. Phys. 29, 383.

129. E. O. Stejskal and H. S. Gutowsky, J. Chem. Phys. 28, 388.

130. G. H. Stewart and H. Eyring, J. Chem. Ed. 35, 550.

131. J. D. Swalen and B. P. Stoicheff, J. Chem. Phys. 28, 671.

132. P. H. Verdier and E. B. Wilson, Jr., J. Chem. Phys. 29 340.

1959

131a. H. C. Allen and E. K. Plyler, J. Chem. Phys. 31, 1062.

132a. R. F. Curl, Jr., J. Chem. Phys. 30, 1529.

133. A. Danti and J. L. Wood, J. Chem. Phys. 30, 582.

134. A. A. Evett, J. Chem. Phys. 31, 1419.

135. G. M. Harris and F. E. Harris, J. Chem. Phys. 31, 1450.

136. D. R. Herschbach, J. Chem. Phys. 31, 91.

137. P. H. Kasai and R. J. Myers, J. Chem. Phys. 30, 1096.

137a. T. Kasuya and T. Oka, J. Phys. Soc. Japan 14, 980.

138. L. C. Krisher and E. B. Wilson, Jr., J. Chem. Phys. 31, 882.

139. V. W. Laurie, J. Chem. Phys. 30, 1210.

140. V. W. Laurie, J. Chem. Phys. 31, 1500.

141. V. W. Laurie and D. R. Lide, J. Chem. Phys. 31, 939.

142. D. R. Lide, Jr., J. Chem. Phys. 30, 37.

142a. D. R. Lide, Jr., Spectrochim. Acta 15, 473

143. D. R. Lide and D. E. Mann, J. Chem. Phys. 31, 1129.

144. C. C. Lin and J. D. Swalen, Rev. Mod. Phys. 31, 841.

145. L. Pierce, J. Chem. Phys. 31, 547.

146. L. Pierce and L. C. Krisher, J. Chem. Phys. 31, 875.

147. L. Pierce and J. M. O'Reilly, J. Mol. Spectroscopy 3, 536.

149. J. D. Swalen and C. C. Costain, J. Chem. Phys. 31, 1562.

150. W. Weltner, J. Chem. Phys. 31, 264.

151. E. B. Wilson, Jr., "The Problem of Barriers to Internal Rotation in Molecules," Advances in Chemical Physics 2, 367 (Interscience Publishers, Inc., New York, 1959).

1960

152. B. Bak, S. Detoni, L. Hansen-Nygaard, J. T. Nielsen and J. Rastrup-Andersen, Spectrochim. Acta 16, 376.

153. D. G. Burkhard, J. Opt. Soc. Am. 50, 1214.

154. W. L. Clinton, J. Chem. Phys. 33, 632.

154a. H. G. Hecht, D. M. Grant, and H. Eyring, Mol. Phys. 3, 577.

155. M. Karplus, J. Chem. Phys. 33, 316.

156. L. C. Krisher and L. Pierce, J. Chem. Phys. 32, 1619.

157. L. C. Krisher, J. Chem. Phys. 33, 304.

158. L. C. Krisher, J. Chem. Phys. 33, 1237.

159. T. Kojima, J. Phys. Soc. Japan 15, 284.

160. T. Kojima, J. Phys. Soc. Japan 15, 1284.

161. V. W. Laurie, J. Chem. Phys. 32, 1588.

162. D. R. Lide, Jr., J. Chem. Phys. 33, 1514.

163. D. R. Lide, Jr., J. Chem. Phys. 33, 1519.

163a. J. T. Massey, C. I. Beard, and C. H. Jen, J. Mol. Spectroscopy 5, 405.

164. R. J. Myers and E. B. Wilson, J. Chem. Phys. 33, 186.

165. L. Pierce and D. H. Petersen, J. Chem. Phys. 33, 907.

166. H. D. Rudolph, H. Dreizler, and W. Maier, Z. Naturforschg. 15a, 742.

1961

167. P. Cahill and S. Butcher, J. Chem. Phys. 35, 2255.

168. W. B. Dixon and E. B. Wilson, Jr., J. Chem. Phys. 35, 191.

169. H. Dreizler, Z. Naturforschg. 16a, 1354.

170. W. G. Fateley and F. A. Miller, Spectrochim. Acta 17, 857.

171. M. Hayashi and L. Pierce, J. Chem. Phys. 35, 1148.

172. T. Kojima, E. L. Breig, and C. C. Lin, J. Chem. Phys. 35, 2139.

173. V. W. Laurie, J. Chem. Phys. 34, 1516.

174. W. F. Libby, J. Chem. Phys. 35, 1527.

175. D. R. Lide, Jr., and D. Christensen, J. Chem. Phys. 35, 1374.

176. J. M. O'Reilly and L. Pierce, J. Chem. Phys. 34, 1176.

177. L. Pierce, J. Chem. Phys. 34, 498.

178. L. Pierce and M. Hayashi, J. Chem. Phys. 35, 479.

179. M. L. Sage, J. Chem. Phys. 35, 142.

180. K. M. Sinnott, J. Chem. Phys. 34, 851.

1962

181. B. Bak, D. Christensen, J. Christensen, L. Hansen-Nygaard, and J. Rastrup-Andersen, Spectrochim. Acta 18, 1421.

182. R. A. Beaudet and E. B. Wilson, Jr., J. Chem. Phys. 37, 1133.

183. W. G. Fateley and F. A. Miller, Spectrochim. Acta 18, 977.

184. E. Hirota, J. Chem. Phys. 37, 283.

185. T. Kasuya, Sci. Papers Inst. Phys. and Chem. Research (Tokyo, Japan) 56, 1.

186. V. Magnasco, Nuovo Cimento 24, 425.

187. W. Maier, Pure and App. Chem. 4, 157.

188. K. D. Möller and H. G. Andresen, J. Chem. Phys. 37, 1800.

189. L. J. Nugent and C. D. Cornwell, J. Chem. Phys. 37, 523.

189a. R. L. Redington, W. B. Olsen, and P. C. Cross, J. Chem. Phys. 36, 1311.

190. H. D. Rudolph, Z. Naturforschg. 17a, 288.

191. R. H. Schwendeman and G. D. Jacobs, J. Chem. Phys. 36, 1245.

192. R. H. Schwendeman and G. D. Jacobs, J. Chem. Phys. 36, 1251.

193. E. B. Wilson, Jr., Pure and App. Chem. 4, 1.

Papers in press, abstracts of recent talks, and private communications:

194. R. A. Beaudet, J. Chem. Phys. (in press).

195. S. Butcher, Paper C9, Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June, 1961.

196a. W. G. Fateley and F. A. Miller, Paper C408, International Symposium on Molecular Structure and Spectroscopy, Tokyo, Japan, September, 1962.

196. E. Hirota, J. Chem. Phys. (in press); Paper F6, Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June, 1962; Paper C402, International Symposium on Molecular Structure and Spectroscopy, Tokyo, Japan, September, 1962.

196b. B. Kirtman, J. Chem. Phys. (in press).

197. V. W. Laurie, Private Communication.

198. D. H. Petersen and L. Pierce, Paper N10, Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June, 1960.

199. L. Pierce and M. Hayashi, Paper F10, Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June, 1962, and private communication.

200. L. Pierce and C. R. Nelson, Private Communication.

201. J. Rigden, Paper C3, Symposium on Molecular Structure and Spectroscopy, Columbus, Ohio, June, 1961; and private communication.