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BIBLIOGRAPHY FOR HINDERED INTERNAL ROTATION
AND MICROWAVE SPECTROSCOPY

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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

$$V(\alpha) = \frac{1}{2}V_N(1-\cos N\alpha) + \frac{1}{2}V_{2N}(1-\cos 2N\alpha) + \dots, \quad (1)$$

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 $\pm 5\%$. 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	ν_3^a	Other Data ^a	References ^b
		C-C Bonds ~~~~~		
CH ₃ CH ₃	ethane	2.9 ^{c,d}	I	<u>31</u> ,123,131 [*]
CH ₃ CH ₂ F	ethyl fluoride	3.31	I,ETS	64,80,132, 152 [*]
CH ₃ CHF ₂	1,1-difluoro- ethane	3.18	ETS	53, <u>80</u>
CH ₃ CF ₃	methyl fluoro- form	3.5 ^e	I,ETS	19, <u>29</u>
CH ₂ FCF ₃	1,1,1,2-tetra- fluoroethane	4.2 ^d		133
CH ₃ CH ₂ Cl	ethyl chloride	3.69	I,ETS	55,74,115, <u>142</u> , <u>191</u> [*]
CH ₃ CH ₂ Br	ethyl bromide	3.57	I,ETS	75,116, <u>142</u>
CH ₃ CH ₂ I	ethyl iodide	2.4 ^f		137a
CH ₃ CH ₂ CN	ethyl cyanide	3.05	ETS,EVS	105, <u>141</u>
CH ₃ CH ₂ CH ₃	propane	>2.7	I	162
CH ₃ CH ₂ SiH ₃	ethyl silane	2.65	I,ETS	198
c-CH ₃ CH ₂ CHO	<u>cis</u> -propion- aldehyde	2.7		193,195
CH ₃ CH ₂ CH ₂ F	propyl fluoride			
	<u>trans</u> isomer	2.69	ETS	184
	<u>gauche</u> isomer	2.87	EVS	
(CH ₃) ₃ CH	isobutane	3.9 ^e	I,ETS,EVS	125,163 [*]
(CH ₃) ₃ CF	t-butyl fluoride	4.3 ^e	ETS	125
CH ₃ CHO	acetaldehyde	1.17	I	85, <u>98</u> [*] ,132, <u>136</u>
CH ₃ COF	acetyl fluoride	1.04	I	146
CH ₃ COCl	acetyl chloride	1.30	I	180
CH ₃ COBr	acetyl bromide	1.30	I	158
CH ₃ COCN	acetyl cyanide	1.27	I	138,157
CH ₃ COOH	acetic acid	0.48	I	114

Formula	Compound	V_3^a	Other Data ^a	References ^b
$(CH_3)_2CO$	acetone	0.76	I	149
$CH_3COC_2H_5$	<u>cis</u> -butanone	0.50	I	200
$CH_3CH=CH_2$	propylene	1.98	I	107,121,175*
$t-CH_3CH=CHF$	<u>trans</u> 1-fluoro-propene	2.15		111
$c-CH_3CH=CHF$	<u>cis</u> 1-fluoro-propene	1.06		182
$CH_3CF=CH_2$	2-fluoro-propene	2.44	ETS	147
$t-CH_3CH=CHCN$	<u>trans</u> -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_3CH-CH_2 $\diagup$ $\diagdown$ O	propylene oxide	2.56	ETS	112,122
$c-CH_3CH-CHCH_3$ $\diagdown$ $\diagup$ O	<u>cis</u> 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, <u>65</u> , 90

Other C-IV Bonds
~~~~~

CH_3SiH_3	methyl silane	1.66	I, ETS, NR	23, 47, <u>99</u> * 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, <u>32</u>

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, <u>139*</u>
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, <u>106*</u> , <u>110</u>
$(CH_3)_2NH$	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 di-fluoroarsine	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 hypo-chlorite	>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
$(\text{CH}_3)_2\text{O}$	dimethyl ether	2.72		137
$t\text{-CH}_3\text{OC}_2\text{H}_5$	ethyl methyl ether	2.53	I, ETS	199
CH_3SH	methyl mercaptan	1.27	I, ETS, NR	60, 63, 69, 103, <u>160</u>
$(\text{CH}_3)_2\text{S}$	dimethyl sulfide	2.10	I, ETS	166, <u>178*</u> , 190

Sixfold Barriers

V_6
(cal/mole)

CH_3BF_2	methyl boron difluoride	13.77		109
CH_3NO_2	nitromethane	6.03	I	58, <u>89</u>

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

^aValues 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).

^bSee 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.

^cFrom thermodynamic measurements.

^dFrom infrared spectroscopy.

^eFrom microwave intensity measurements.

^fThe reported value is probably quite inaccurate.

Table II. Barrier heights (kcal/mole).

C-C Bonds					
CH ₃ CH ₃	2.9 ^a	CH ₃ CHO	1.17	CH ₃ CH=CH ₂	1.98
CH ₃ CH ₂ F	3.31	CH ₃ COF	1.04	t-CH ₃ CH=CHF	2.15
CH ₃ CHF ₂	3.18	CH ₃ COCl	1.30	t-CH ₃ CH=CHCl	2.17
CH ₃ CF ₃	3.5 ^b	CH ₃ COBr	1.30	c-CH ₃ CH=CHF	1.06
CH ₃ CH ₂ Cl	3.56	CH ₃ COCN	1.27	CH ₃ CF=CH ₂	2.44
CH ₃ CH ₂ Br	3.57	CH ₃ COOH	0.48	t-CH ₃ CH=CHCN	>2.1
CH ₃ CH ₂ CN	3.05	(CH ₃) ₂ CO	0.76	CH ₃ CH=C=O	1.20
CH ₃ CH ₂ CH ₃	>2.7	CH ₃ COC ₂ H ₅	0.50	CH ₃ CH=C=CH ₂	1.59
CH ₃ CH ₂ SiH ₃	2.65			(CH ₃) ₂ C=CH ₂	2.21
c-CH ₃ CH ₂ CHO	2.7			CH ₃ CH-CH ₂	2.56
t-CH ₃ CH ₂ CH ₂ F	2.69			c-CH ₃ CH-CHCH ₃	1.61
g-CH ₃ CH ₂ CH ₂ F	2.87			CH ₃ C≡CCH ₂ Cl	<0.050
(CH ₃) ₃ CH	3.9 ^b				
(CH ₃) ₃ CF	4.3 ^b				
Other C-IV Bonds		C-V Bonds		C-VI Bonds	
CH ₃ SiH ₃	1.66	CH ₃ NH ₂	1.98	CH ₃ OH	1.07
CH ₃ SiH ₂ F	1.56	(CH ₃) ₂ NH	3.4 ^a	CH ₃ OCl	>3
CH ₃ SiHF ₂	1.26	(CH ₃) ₃ N	4.4 ^b	CH ₃ OOCH	1.19
CH ₃ SiF ₃	1.2 ^b	CH ₃ PH ₂	1.96	CH ₃ ONO ₂	2.32
(CH ₃) ₂ SiH ₂	1.67	(CH ₃) ₂ PH	2.20	(CH ₃) ₂ O	2.72
(CH ₃) ₃ SiH	1.8 ^b	(CH ₃) ₃ P	2.6 ^b	t-CH ₃ OC ₂ H ₅	2.53
SiH ₃ C ₂ H ₅	1.98	CH ₃ AsF ₂	1.33	CH ₃ SH	1.27
SiH ₃ CH ₂ Cl	2.55	(CH ₃) ₃ As	2 ^b	(CH ₃) ₂ S	2.10
SiH ₃ CH ₂ =CH ₂	1.50				
CH ₃ GeH ₃	1.24				
CH ₃ SnH ₃	0.65				
Sixfold Barriers (cal/mole)					
		CH ₃ BF ₂	13.77		
		CH ₃ NO ₂	6.03		
		CD ₃ NO ₂	5.19		

^aFrom thermodynamic data or infrared spectra.

^bFrom microwave intensity measurements.

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

Molecule	V ₃	V ₆	V ₆ /V ₃	Ref.
CH ₃ CH ₂ Cl	3.69±0.30	0±0.003	~0%	196a
	3.69±0.10			191
CH ₃ CH=CH ₂	2.03±0.30	-0.045±0.003	-2.3%	196a
	1.98±0.17			107
CH ₃ CF=CH ₂	2.34±0.10	0.011±0.003 <0.050	0.6% <2.5	196a
	2.46±0.05			147
CH ₃ CH-CH ₂ O	2.58±0.23	-0.026±0.003 <0.030	-1.0% <1%	196a
	2.56±0.72			122

^aThe 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/mol).

Formula	Compound	Reference

$\text{CH}_3\text{CH}_2\text{CH}_2\text{F}$	n-propyl fluoride	184

$$V(\alpha) = \sum_n \frac{1}{2} V_n (1 - \cos n\alpha)$$

Trans

Gauche

Cis

Formula	Compound	Reference
$\text{CH}_2\text{FCH}=\text{CH}_2$	allyl fluoride	196

$\text{C}_6\text{H}_5\text{OH}$	phenol	159

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

$$V_2 = 3.15 \pm 0.3$$

$$\alpha = 0^\circ, 180^\circ \text{ for planar configuration}$$

Formula	Compound	Reference
NH_2NH_2	hydrazine	185
$V(\alpha) = \frac{1}{2}V_2(1+\cos 2\alpha)$		
$V_2 = 3.15 \pm 0.15$		
$V_2 = V_{\text{cis}} = V_{\text{trans}} \text{ assumed}$		
$\alpha \approx 90^\circ \text{ at potential minimum}$		

Cis ($\alpha=0^\circ$)

Trans ($\alpha=180^\circ$)

NF_2NF_2	tetrafluorohydrazine	143
$V_2 > 3$		
$\alpha \approx 65^\circ \text{ at potential minimum}$		

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

$$V_0 = 1.22$$

$$V_1 = 2.86$$

$$V_2 = 2.15$$

Cis

$\alpha = 109.5^\circ$ at potential minimum
 $\langle \alpha \rangle =$ average dihedral angle
 $= 119.8^\circ$

Trans

Table V. Equilibrium configurations.

Compound	Configuration	References
<u>C-C Bonds</u>		
$\text{CH}_3\text{CH}_2\text{F}$	Staggered	152
$\text{CH}_3\text{CH}_2\text{Cl}$	Staggered	74
$\text{CH}_3\text{CH}_2\text{CH}_3$	Both methyl groups staggered with respect to methylene group	162
$(\text{CH}_3)_3\text{CH}$	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
$\text{CH}_3\text{CH}=\text{CH}_2$	Methyl group eclipses double bond and staggers methine H	121
$(\text{CH}_3)_2\text{C}=\text{CH}_2$	Both methyl groups eclipse double bond	173
<u>Other C-IV Bonds</u>		
CH_3SiH_3	Staggered	99
$\text{CH}_3\text{SiH}_2\text{F}$	Staggered	128
CH_3SiHF_2	Staggered	156
$(\text{CH}_3)_3\text{SiH}$	Each methyl group staggered with respect to siline group	165

Compound	Configuration	References
$\text{SiH}_3\text{CH}=\text{CH}_2$	Silyl group staggered with respect to methine group	176
CH_3GeH_3	Staggered	139
<u>C-VI Bonds</u>		
CH_3OOCH	Methyl group staggered with respect to formyl group	132a
$\text{C}_6\text{H}_5\text{OH}$	Planar	159
$(\text{CH}_3)_2\text{S}$	Both methyl groups staggered with respect to the adjacent CS bond	178
<u>Other Bonds</u>		
NH_2NH_2	Dihedral angle = 90°	185
NF_2NF_2	Dihedral angle = 65°	143
H_2O_2	Dihedral angle = 120°	189a
<u>Rotational Isomers</u>		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{F}$	Gauche configuration of CH_3 and F slightly more stable than trans	184
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CN}$	Gauche configuration of CH_3 and CN slightly more stable than trans	196
$\text{CH}_2\text{FCH}=\text{CH}_2$	Cis configuration of F and $\text{C}=\text{CH}_2$ group slightly more stable than trans	196

Table VI. Angles of tilt.

Molecule	Bond	θ^a	Reference
$(\text{CH}_3)_2\text{SiH}_2$	C-Si	0°	177
CH_3NH_2	C-N	3°	106
CH_3OH	C-O	5°	94
$(\text{CH}_3)_2\text{O}$	C-O	5°	137
CH_3SH	C-S	2.5°	160
$(\text{CH}_3)_2\text{S}$	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 $\pm 1^\circ$.

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 9(1)14	0(1)100 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

^aFor notation see, for example, reference 136.

^bA close tabulation is given for low s values.

^cEigenfunctions are also tabulated.

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

^ePerturbation coefficients and matrix elements
required for the treatment of coupling of internal
and over-all rotation are tabulated.

^fRelations 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

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