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RESEARCH AND
DEVELOPMENT
REPORT

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Physics (UC-34)

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UNITED STATES ATOMIC ENERGY COMMISSION

Research and Development Report

CATALOG OF NUCLEAR QUADRUPOLE
INTERACTIONS AND RESONANCE FRE-
QUENCIES IN SOLIDS. PART II.
HALOGEN RESONANCES IN ORGANIC
COMPOUNDS

by

S. L. Segel and R. G. Barnes

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IN NUCLEAR SCIENCE ABSTRACTS

September, 1965

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TABLE OF CONTENTS

	Page
ABSTRACT	vii
INTRODUCTION	vii
ELEMENTS OF PURE NUCLEAR QUADRUPOLE RESONANCE THEORY	ix
Pure Quadrupole Transition Frequencies	xi
TABLE OF ALTERNATIVE NUCLEAR SPECIES	xiii
EXPLANATORY NOTES	xiii
CATALOG	
CHLORINE (35) RESONANCES	
Acetanilides	1
Aldehydes	2
Aliphatics (other than alkyl)	3
Aliphatic acids and derivatives	5
Alkyl, chloromethanes	7
Alkyl, chloroethanes	8
Alkyl, chloropropanes	10
Alkyl, chlor-anes (higher than propanes)	11
Anilines	13
Anisoles and phenetoles	14
Benzoic acids and derivatives	15
Carbonyl chlorides	16
Chlorobenzenes	18
Heterocyclics and polyheterocyclics	20
Homocyclics and polyhomocyclics (this includes all single ring compounds, both aromatic and non-aromatic, which do not fall into other specified classes)	
Ketones (Aliphatic)	24
Ketones (Aromatic)	25
Nitriles, isocyanates, and thiazoles.	26
Nitrobenzenes	27
Nitrogen mustards	28

Phenols	29
Pyridines and pyrimidines	31
Quinolines, quinones and derivatives	33
Silanes	35
Sulfonic acids and salts and sulfinates	37
Sulfonyl chlorides	38
Toluenes and xylenes	39
BROMINE (79) and (81) RESONANCES	
Acetanilides	40
Aliphatic acids and derivatives	41
Alkyl, bromomethanes	42
Alkyl, bromoethanes	43
Alkyl, bromopropanes	44
Alkyl, bromo-anes (higher than propanes)	45
Anilines	46
Anisoles and phenetoles	47
Benzoic acids and derivatives	48
Brombenzenes	49
Carbonyl Bromides	50
Homocyclics and multicyclics and heterocyclics	51
Ketones	54
Nitrobenzenes	55
Phenols	56
Pyridines and pyrimidines	57
Quinones and quinolines	58
IODINE (127) RESONANCES	
Alkyl, iodomethanes	59
Alkyl, iodoethanes	60
Alkyl, iodopropanes	61
Alkyl, iodo-anes (higher than propanes)	62
Anilines	63
Anisoles and phenetoles	64
Nenzoic acids and derivatives	65
Homocyclics, heterocyclics and aliphatics	66

Iodobenzenes	67
Nitrobenzenes	68
Phenols	69
Toluenes and xylenes	70
REFERENCES	R1

IS-1222

IS-1222

CATALOG OF NUCLEAR QUADRUPOLE INTERACTIONS AND
RESONANCE FREQUENCIES IN SOLIDS. PART II.
HALOGEN RESONANCES IN ORGANIC COMPOUNDS

S. L. Segel and R. G. Barnes

ABSTRACT

Where available in literature, the halogen quadrupole resonance frequencies and the coupling constants in organic compounds are listed. The sources of the information are the more commonly available journals through August, 1965. Literature references to the original sources are given as well as references to articles immediately concerned with the quadrupolar coupling. A brief introduction to the theory of quadrupole resonance is also given.

INTRODUCTION

The basic purpose underlying the preparation of this catalog of nuclear quadrupole resonance data has been to provide easy access to the rather large body of experimental data that has been accumulated. The information immediately available in this catalog is the quadrupole resonance frequency for a given nucleus in a given compound, and, where reported in the literature, the coupling constant. For those cases where the coupling constant is not given, we have provided the equations which enable one to calculate them. In addition, we have provided a listing of quadrupole moment ratios which enable one to calculate the coupling constant for a different isotope than the one listed in the catalog.

This part of the catalog is restricted to halogen resonances in organic compounds. Resonances in elements and inorganic compounds is dealt with in Part I. Inspection of the contents on pages iii, iv, and v, of this catalog reveals the scope and delineation of the classes of organic compounds. Subsequent pages will give the ELEMENTS OF PURE NUCLEAR QUADRUPOLE RESONANCE THEORY and other details such as how the listing can be most easily used.

Due to the complexities of any tabulation of organic compounds, this particular system was developed keeping in mind the number of compounds observed in a given class, the interest of a given class, and the probability that more compounds in this class would be investigated. One should be familiar with groupings in the table of contents as well as with the supplementary guides following the listings.

Only in a few instances are compounds cross-indexed. If a given compound has none of the characteristic groups in the listing, it can be found in the homocyclic or heterocyclic group. All other characteristic groups take precedence in nomenclature over the nitro group except for homo- and heterocyclic. Some illustrative examples are:

- a) parachloro-phenoxyacetic acid; since there is no listing for the aromatic acetic acids and this is a single ring compound, it will be found in the homocyclic group.
- b) p-chlorophenetole; the phenetoles are listed with the anisoles.
- c) chloral hydrate; the -al suffix implies that it is an aldehyde.

Knowing the formula helps.

- d) chloroacetal; not really an aldehyde, not alkyl. Look under aliphatic.
- e) N-chloro-p-quinoneimide; see under quinones and derivatives.

ELEMENTS OF PURE NUCLEAR QUADRUPOLE RESONANCE THEORY

The electrical interaction between an atomic nucleus and its surrounding electronic charge distribution can be expressed in a series corresponding to the effects of various electrical multipoles. In this series the first term represents the interaction of a point charge with the electronic field while the second and third terms describe electric quadrupole and hexadecapole interactions. The latter two terms are relevant only when the nuclear shape departs from spherical symmetry. In addition, the symmetry properties of the nuclear wave function require that in order for a nucleus to possess an electric quadrupole moment, the spin I must equal or exceed unity (i. e., $I \geq 1$), and that in order for it to possess a hexadecapole moment, it must have $I \geq 2$. Nuclei do not possess electric dipole or octupole moments. Hereafter, we shall only be concerned with the electrical quadrupole interaction.

The quadrupole moment Q interacts with the gradient of the electric field at the position of the nucleus. In general, this field gradient arises from the bonding electrons on the atom, from point charges (ions) external to the atom, and in the case of metals, from

the non-s part of the conduction electron wave function. This gradient is a tensor quantity, $\partial E_i / \partial x_j$, whose elements are determined by the structure and symmetry properties of the solid. Normally, the elements of the field gradient tensor are referred to its principal axis system, so that only the three diagonal elements are needed, $\partial E_x / \partial x$, $\partial E_y / \partial y$ and $\partial E_z / \partial z$. The sum of these three elements, however, satisfies Laplace's equation (excluding the nuclear charge at the origin), so that only two quantities are required to specify the field gradient tensor. These two are conventionally taken to be the principal value of the gradient (the largest element in the principal axis system) which is called $\partial E_z / \partial z = -q$, and the asymmetry parameter η defined by:

$$\eta = [(\partial E_x / \partial x) - (\partial E_y / \partial y)] / (\partial E_z / \partial z) .$$

In all cases, $1 \geq |\eta| \geq 0$.

The Hamiltonian operator for the interaction of the nuclear quadrupole moment with the electric field gradient can be written as:

$$H_Q = [e^2 q Q / 4I(2I - 1)] [(3I_z^2 - I^2) + (\eta/2)(I_+^2 + I_-^2)] .$$

Here, I is the nuclear spin operator with components I_z , I_x , and I_y , and $I_{\pm} = I_x \pm i I_y$. Using the angular momentum eigenfunctions, the energy levels for a given value of I can be worked out by perturbation theory methods. In the special case that $\eta = 0$, the energy levels are given directly by the formula:

$$E_m = [e^2 q Q / 4I(2I - 1)] [3m^2 - I(I + 1)] .$$

Ordinarily, the quantities of direct experimental interest are the transition frequencies between the levels determined by H_Q . These transitions are listed below in frequency units as functions of $e^2 qQ$ and η for half-integral spin values. The quantity $e^2 qQ$ is the so-called "quadrupole coupling constant", and is usually expressed in frequency units. In the important case of spin $3/2$, the single transition frequency does not permit $e^2 qQ$ and η to be separately determined. However, because the effect of η on the transition frequency is relatively small in this case, the coupling constant is often taken for simplicity to be twice the transition frequency.

Pure Quadrupole Transition Frequencies:

$$I = 3/2: \quad \nu = (e^2 qQ/2h)(1 + \eta^2/3)^{1/2}.$$

$$I = 5/2: \quad \begin{aligned} \nu_1 &= (3/20)(e^2 qQ/h)(1 + 0.0926\eta^2 - 0.634\eta^4) \\ \nu_2 &= (6/20)(e^2 qQ/h)(1 - 0.2037\eta^2 + 0.162\eta^4). \end{aligned}$$

In the limit of zero asymmetry parameter, the transition frequencies follow in the simple ratios of small numbers, 1:2. In those cases where two isotopes of the same element have the same spin, the ratios of the quadrupole resonance frequencies will be the same as the ratio of the quadrupole coupling constants.

The above formulas for the transition frequencies become inappropriate when η becomes moderately large. In such cases, the matrix of the Hamiltonian H_Q must be diagonalized exactly by numerical methods to obtain the energy levels and transitions. Several calculations of this type have been made and published, as follows:

R. Livingston and H. Zeldes, Table of Eigenvalues for Pure Quadrupole Spectra, Spin $5/2$, U. S. A. E. C., ORNL - 1913 (1955). This tabulation gives the energy eigenvalues for increments of 0.001 η between 0 and 1.

M. H. Cohen, Phys. Rev. 96, 1278 (1954). This paper gives the energy eigenvalues for spins $5/2$, $7/2$, and $9/2$ for increments of 0.1 in η between 0 and 1.

Finally, for convenience, we include here a short listing of references to the subject of nuclear quadrupole resonance spectra, some of which are of a general, review nature, while others are of historical interest:

R. V. Pound, Phys. Rev. 79, 685 (1959).

C. H. Townes and B. P. Dailey, J. Chem. Phys. 17, 782 (1949); 20, 35 (1952).

R. Bersohn, J. Chem. Phys. 20, 1505 (1952).

M. H. Cohen and H. Reif, Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1957), Vol. 5, Chapter 5.

T. P. Das and E. L. Hahn, Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1957), Supplement I.

A. Abragam, The Principles of Nuclear Magnetism (Oxford University Press, London, 1961), Chapter VII.

V. Rehn, Jour. Chem. Phys. 38, 749 (1963).

R. Dixon, Jour. Chem. Phys. 41, 1720, 1739 (1964) [Electrically Induced Perturbation of Quadrupole Interaction]

TABLE OF ALTERNATIVE NUCLEAR SPECIES

Nuclear species used in catalog	Alternative abundant isotope	Quadrupole moment ratio ^a
Cl ³⁵	Cl ³⁷ : I = 3/2 , 25%	$Q^{35}/Q^{37} = 1.26878$
Br ⁷⁹	Br ⁸¹ : I = 3/2 , 49.4%	$Q^{79}/Q^{81} = 1.19707$
I ¹²⁷	100%	

^aC. H. Townes, Handbuch der Physik, edited by S. Flügge (Springer Verlag, Berlin, 1958), Vol. 38, p. 444.

EXPLANATORY NOTES

For the most part the column headings are self-explanatory. Under the heading ISO or ν we have provided space for denoting the particular transition in those cases where a nuclear species has more than two quadrupole levels. The designation of these transitions (1, 2) is that commonly used in the literature, and the explicit expressions for these transitions for the various spin values are given in the brief THEORY section of this catalog. In addition, there are instances when the literature reference concerns an isotope different from the one used in the catalog classification (e. g., BR(81) instead of Br(79)). This column is then used to note that the data apply to the different isotopes. When this column contains neither transition numbers nor isotopic designation but several resonance frequencies are given, these are due to the presence of non-equivalent sites in the solid (see THEORY).

In those cases where the coupling constant is given, the coupling constant applies at the temperature for which the frequency is given.

If resonance frequencies are given for more than one temperature, the temperature for which the coupling constant applies is stated.

The abbreviations used in the REFERENCES column have the following meanings:

- F Basic frequency reference for pure nuclear quadrupole experiments and for the quadrupole coupling if this were based on other methods (e. g., nuclear magnetic resonance).
- P References to pressure dependence of frequency or coupling constant.
- R References to measurements of relaxation times.
- S References to measurements of line width and shape and to experiments which alter these quantities, such as impurities and radiation damage.
- T References to temperature dependence of frequency or coupling constant.
- Z References to the Zeeman effect in pure nuclear quadrupole resonance and to cases where the quadrupole coupling was determined from magnetic resonance experiments. In almost all cases where the same literature reference is listed under both the F and Z categories the quadrupole coupling has been determined from magnetic resonance experiments.

Acetanilides

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
M-chloroacetanilide M-Cl $\emptyset$ NHCOCH ₃	34.735					F(B12)
O-chloroacetanilide O-Cl $\emptyset$ NHCOCH ₃	35.150					F(B2)
P-chloroacetanilide P-Cl $\emptyset$ NHCOCH ₃	34.792					F(B12)
2,5-dichloroacetoacetanilide 2,5-Cl ₂ $\emptyset$ NHCOCH ₂ COCH ₃	35.000 35.232					F(B12)

Aldehydes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Para-chlorobenzaldehyde $\text{P-Cl } \phi \text{ CHO}$	34.607 34.623					F(M1)
5-chloro-2-hydroxy- benzaldehyde	34.968					F(B12)
Chloro-paraldehyde $(\text{CH}_2\text{ClCHO})_3$	35.363 35.691					F(A1, A2)
Chloral alcoholate(methyl) $\text{CCl}_3\text{CH}(\text{OH})(\text{OCH}_3)$			38.59 38.74 38.83	90°K		F(T3)
Chloral alcoholate(ethyl) $\text{CCl}_3\text{CH}(\text{OH})(\text{OC}_2\text{H}_5)$	38.516 38.705 39.140					F(T3, B3)
Chloral hydrate $\text{CCl}_3\text{CH}(\text{OH})_2$	38.190 39.429 39.515					F(A1, A2)
2, 4-dichlorobenzaldehyde	35.461 35.986					F(H8)
3, 4-dichlorobenzaldehyde	35.585 36.762					F(H8)

Aliphatics (other than alkyl)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2, 2, 2-trichloroethoxy ethanol	38.516 38.705 39.140					F(B3, T3)
α -chloroacetamide $\text{CH}_2\text{ClCONH}_2$	34.889					F(B16, A1, G14, A2); T(G14)
α, α -dichloroacetamide $\text{CHCl}_2\text{CONH}_2$	37.238 37.750					F(M2, G14); T(G14)
2-chloroethyl dimethylamine hydrochloride $\text{ClCH}_2\text{CH}_2\text{N}(\text{CH}_3)_2 \cdot \text{HCl}$	35.0					F(B16)
2-chloroethyl dimethylamine hydrochloride $\text{ClCH}_2\text{CH}_2\text{N}(\text{C}_2\text{H}_5)_2 \cdot \text{HCl}$	34.7					F(B16)
Chloroacetal $\text{ClCH}_2\text{CH}(\text{OCH}_3)_2$	34.608					F(B16)
Chloropicrin CCl_3NO_2	41.003 41.235 41.546					F(B16)
Dichloro-diethyl carbonate (β, β') $(\text{ClCH}_2\text{O})_2\text{CO}$	33.775 34.312					F(B16)
Trichloroacetamide $\text{CCl}_3\text{CONH}_2$	38.850 39.478 39.599 39.665 39.817 40.007					F(A1, A2, G14); T(A2, G14)
Sym dichloro-dimethyl ether $\text{CH}_2\text{Cl}-\text{O}-\text{CH}_2\text{Cl}$	32.381 32.587					F(L1)
Chloromethyl methyl ether	29.817 30.206					F(H8)

Aliphatics (cont.)

COMPOUND	FREQ. AT 77°K.	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCE
Allyl chloride CH_2CHCHCl	33.455					F(H8)
3-chloropropyne	35.812					F(H8)
1,4-dichloro-2-butene	34.109					F(H8)
Perchloroethylene	38.342 38.526 38.648 38.799					F(H8)
Bis(2-chloroethyl)ether	33.997 33.391					F(H8)
1,2-bis(2-chloroethoxy)-ethane	33.932 33.724 33.249					F(H8)
CCl_3SCl	39.166 39.827 40.117					F(H8)
Butyl chloral hydrate	37.425 36.954 35.017					F(H8)

Aliphatic Acids and Derivatives

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Chloroacetic acid CH_2ClCOOH	36.131 36.429					F(A1, A2, N3, B26); Z(G15)
Dichloroacetic acid CHCl_2COOH	37.979 38.807					F(A1, A2)
Trichloroacetic acid CCl_3COOH	39.967 40.165 40.240					F(A1, A2)
Ethyl chloroacetate $\text{CH}_2\text{ClCOOC}_2\text{H}_5$	35.962					F(A1, A2)
Sodium chloroacetate $\text{CH}_2\text{ClCOONa}$	34.794					F(A1, A2)
Phenylchloroacetate $\text{CH}_2\text{ClCOO} \phi$	36.172 36.386 36.430 36.897					F(B16)
Methyl dichloroacetate $\text{CHCl}_2\text{COOCH}_3$	37.306 37.351 37.385 37.621 37.828 38.334 38.724					F(B16)
Ethyl trichloroacetate $\text{CCl}_3\text{COOC}_2\text{H}_5$	40.200 40.339					F(W4)
Ethyl chloroformate $\text{ClCOOC}_2\text{H}_5$	33.858					F(B9, W4)
2-chloroethyl acetate $\text{CH}_3\text{COOC}_2\text{H}_4\text{Cl}$	34.104					F(H8)

Aliphatic acids (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
M-butyl chloroacetate $\text{CH}_2\text{ClOOC}_4\text{H}_9$	36.363 36.136					F(H8)
β -chloropropionic acid $\text{C}_2\text{H}_4\text{ClOOH}$	33.953					F(H8)
Methyl trichloroacetate $\text{CCl}_3\text{COOCH}_3$	40.152 39.867 39.763 39.681					F(H8)
Muchochloric acid	37.344 36.576					F(H8)

Alkyls, Chloromethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
CCl_4	40.6*					F(L1, L5, L9, R1, D36); S(D24); T(G7)
CHCl_3	38.354 38.308					F(L1, L3, L5, L9, R1, G6, D36); T(G7)
CH_2Cl_2	35.991					F(L1, L3, L5, L9, D36, R1, G6); T(G7)
CH_3Cl	34.029					F(L1, L5, W6, D36, L9, K21, R1, G6); S(D24)
CFCl_3	39.161 39.517 39.703					F(L9)
CF_2Cl_2	38.450					F(L1, L9)
CF_3Cl	38.089					F(L1, L9, R1)
CHFCl_2	36.479 36.508					F(L9)
CH_2FCl			33.799	20°K		F(L1, L2)
CHF_2Cl			35.249	20°K		F(L9)
CBrF_2Cl	38.342					F(L1, L9)
CCl_3SCl	39.166 39.827 40.117					F(H8)

*average of 12 lines

Alkyls, Chloroethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES	∞
CCl_3CCl_3	40.551 40.685 40.714 40.761					F(L1, L2, L5); T(T6, A12)	
$\text{CCl}_3\text{CHCl}_2$	38.711 38.759 39.758 39.836 39.862					F(L1, L2)	
$\text{CHCl}_2\text{CHCl}_2$	37.481 37.667 37.989					F(B16)	
$\text{CH}_2\text{ClCH}_2\text{Cl}$	34.361					F(L1, L2, D36, D16, W6); T(D14, R13)	
$\text{CH}_3\text{CH}_2\text{Cl}$			32.891 33.080	20°K		F(L2, D36)	
CH_3CHCl_2	35.412					F(L2)	
CH_3CCl_3	37.829 38.052					F(L2, G5, D36); R(G5); T(G7)	
ClCH=CHCl cis			34.968 35.029	20°K		F(L1)	
ClCH=CHCl	35.968					F(L1, W6)	
$\text{CH}_3\text{CCl}(\text{NO}_2)_2$	40.150					F(B16)	

Alkyls, Chloroethanes (cont.)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
$\text{CCl}_3\text{CH}(\text{OH})(\text{OCH}_3)$			37.65 37.80 37.99	13°C		F(T3)
$\text{CCl}_3\text{CH}(\text{OH})(\text{OC}_2\text{H}_5)$	38.516 38.705 39.140		37.80 38.02 38.06	13°C		F(T3, B3)

Alkyls, Chloropropanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
1-Chloropropane	32.968					F(L2, D36)
2-Chloropropane			32.069	20°K		F(L2, D36)
2, 2, -dichloropropane	34.883					F(L1, D36)
1, 2, 3, -trichloropropane			34.677 34.838 35.026			F(L2)
1, 1, 2, 3, 3-pentachloropropane	37.116 37.192 37.588 38.109					F(S4)
Asy. heptachloropropane	39.642 39.792 41.125 41.297 41.429					F(S4)
1, 3-dichloropropane	32.952 33.130					F(H8)
1, 1, 1, 2, 3, 3, 3, -heptachloro- propane	40.200					F(S4, H8)
1, 1, 2, 2, 3, 3-heptachloro- propane	38.267 39.140 39.754 39.900 40.440 41.186 41.276					F(H8)
1-chloro-2-propene	33.455					F(H8)

Alkyl, Chloro-anes (higher than propanes)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Trimethylchloromethane	31.065					F(L2, D36); T(G7)
Trimethyl-ethylchloropropane			30.961	20° K		F(L2)
1,4-dichlorobutane	32.850					F(S4)
1-chloropentane	33.103					F(H8)
1-chlorohexane	32.963					F(H8)
1-chloroheptane	33.106					F(H8)
1-chlorooctane	33.009					F(H8)
1-chlorodecane	33.024					F(H8)
1,5-dichloropentane	33.222					F(H8)
1,6-dichlorohexane	33.008					F(H8)
2-chlorooctane	32.302					F(H8)
1,3-dichlorobutane	31.949 33.485					F(H8)
2,4-dichloropentane	32.686 32.333					F(H8)
2,5-dichlorohexane	31.819					F(H8)
2-chloro-2-methylbutane	30.878					F(H8)
1-chloro-3-methylbutane	32.720					F(H8)
1,1,1,5-tetrachloropentane	38.535 38.038 37.879 33.363					F(H8)

Alkyl, Chloro-anes (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT 1°	TEMP.	COUPLING CONSTANT	REFERENCES
1, 1-dichlorobutane	35.117 35.210					F(H8)
2, 2-dichlorobutane	34.793 34.722					F(H8)
1, 4-dichlorobutane	32.630					F(A10)

Anilines

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
M-chloroaniline	34.388					F(B12)
M-Cl $\emptyset$ NH ₂	34.468					
P-chloroaniline	34.146					F(B22, M1); T(D24); Z(M9, R16)
P-Cl $\emptyset$ NH ₂						
4-chloro-2,6-dinitroaniline	37.280					F(B12)
4-Cl-2,6-(NO ₂) ₂ $\emptyset$ NH ₂						
5-chloro-2-methoxyaniline	34.220					F(B12)
5-Cl-2-OCH ₃ $\emptyset$ NH ₂						
5-chloro-2-methoxyaniline	35.550					F(B16)
hydrochloride						
5-Cl-2-OCH ₃ $\emptyset$ NH ₂ ·HCl						
P-chloro-N,N,-diethylaniline	34.079					F(B12)
P-Cl $\emptyset$ N(C ₂ H ₅) ₂	34.161					
2,4-dichloroaniline	34.734					F(B12)
2,4-Cl ₂ $\emptyset$ NH ₂	34.854					
2,5-dichloroaniline	34.530					F(B3); Z(S38)
2,5-Cl ₂ $\emptyset$ NH ₂	34.413					
3,4-dichloroaniline	35.673					F(B12)
3,4-Cl ₂ $\emptyset$ NH ₂	35.872					
2,6-dichloro-4-nitroaniline	35.524					F(B12)
2,6-Cl ₂ 4-NO ₂ $\emptyset$ NH ₂	35.924					
2,4,6-trichloroaniline	34.925					F(B2, B12)
2,4,6-Cl ₃ $\emptyset$ NH ₂	34.977					
	35.177					
	35.591					
	35.780					
	35.885					

Anisoles and phenetoles

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-chloroanisole P-Cl ϕ OCH ₃	34.753					F(M1)
P-chlorophenetole P-Cl ϕ OC ₂ H ₅	34.381					F(M1)
2,4-dichloroanisole 2,4-Cl ₂ ϕ OCH ₃	35.734 36.256					F(B12)
2,4-dichlorophenetole 2,4-Cl ₂ ϕ OC ₂ H ₅	35.406 36.108					F(B12)
4-chloro-2-aminoanisole 4-Cl-2-NH ₂ ϕ OCH ₃	34.215					F(B12)
β -chlorophenetole ϕ OCH ₂ CH ₂ Cl	34.316					F(B16)

Benzoic Acids and Derivatives

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-chlorobenzoic acid O-Cl ϕ COOH	36.305					F(B1)
M-chlorobenzoic acid MCl ϕ COOH	35.227					F(M1)
P-chlorobenzoic acid P-Cl ϕ COOH	34.673					F(M1); Z(O5)
2-chloro-5-nitro benzoic acid 2-Cl-5-NO ₂ ϕ COOH	37.337					F(B12)
4-chloro-3-nitrobenzoic acid 4-Cl-3-NO ₂ ϕ COOH	37.843					F(B12)
2,4-dichlorobenzoic acid 2,4-Cl ₂ ϕ COOH	35.528 37.432					F(B12)
3,4-dichlorobenzoic acid 3,4-Cl ₂ ϕ COOH	36.576 37.298					F(B12)
M-chlorosulfonyl-benzoic acid M-SO ₂ Cl- ϕ COOH	33.672					F(H8)

Carbonyl Chlorides

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Trichloroacetyl chloride CCl_3COCl	33.721 40.132 40.474 40.613					F(A1, A2, B9, W4)
Dichloroacetyl chloride CHCl_2COCl	32.147 32.962 38.353 38.521 39.189 39.386					F(B9, M2)
Chloroacetyl chloride CH_2ClCOCl	30.437 37.517					F(B9)
Oxalyl chloride ClCOCOCl	33.621					F(B9)
Succinyl chloride $\text{ClCo}(\text{CH}_2)_2\text{COCl}$	30.217					F(B9)
Adipyl chloride $\text{ClCO}(\text{CH}_2)_4\text{COCl}$	28.978					F(B9)
Sebacyl chloride $\text{ClCO}(\text{CH}_2)_8\text{COCl}$	29.118					F(B9)
Fumaryl chloride ClCOCH:CHCOCl	30.380 30.970					F(B9)
2-furoyl chloride	30.726					F(B9)
Anisoyl chloride $\text{CH}_3\text{O} \phi \text{COCl}$	30.09					F(B16)
Benzoyl chloride ϕCOCl	29.93					F(M2)

Carbonyl Chlorides (cont.)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2,4-dichlorobenzoyl chloride $2,4\text{-Cl}_2\text{C}_6\text{H}_3\text{COCl}$	31.039 31.086 35.834 35.923 37.038 37.145					F(B9)
Diphenylcarbamyl chloride $(\text{C}_6\text{H}_5)_2\text{NCOC}_6\text{H}_5$	35.2					F(B16)
Diethylcarbamyl chloride $(\text{C}_2\text{H}_5)_2\text{NCOC}_6\text{H}_5$	31.877					F(B9, M2)
Dimethylcarbamyl chloride $(\text{CH}_3)_2\text{NCOC}_6\text{H}_5$	31.8					F(B9, M2)

Chlorobenzenes

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Chlorobenzene $\text{Cl } \emptyset$	34.622					F(B14, L1, L3, B24); S(D10, M11); T(D24)
O-dichlorobenzene $\text{O-Cl}_2 \emptyset$	35.580 35.755 35.824					F(B14); T(D24)
P-dichlorobenzene * † x $\text{P-Cl}_2 \emptyset$	34.779					F(B22, W6, B14, B24); P(D13, R6, D18, R7, K23, B32); R(W7, S21, G25, W13, H16, B54, B35, T17); S(K15, R6, S18, R7, M12, B31, D19, C16, F2); T(S21, K23, B32, H16, B35, D24); Z(R16, L6, O5, D26, A9, M20, B45, B46)
M-dichlorobenzene $\text{M-Cl}_2 \emptyset$	34.809 34.875 35.030					F(B14)
1, 2, 3-trichlorobenzene $\text{1, 2, 3-Cl}_3 \emptyset$	36.214 36.238 36.268 36.523 36.973 37.031					F(B14); S(T8); T(T8)
1, 2, 4-trichlorobenzene $\text{1, 2, 4-Cl}_3 \emptyset$	35.189 35.617 36.173 36.380 36.400 36.623					F(B14, M3)
1, 3, 5-trichlorobenzene	35.545 35.894 36.115					F(B14); Z(M15, T9)

† Impurity study by B33

x Electric field study by A9, B45, B46

* radiation damage studies by D12, M13, F6

Chlorobenzenes (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
1, 2, 3, 4-tetrachlorobenzene	37.013					F(B14)
1, 2, 3, 4-Cl ₄ $\emptyset$	37.455					
	37.557					
1, 2, 3, 5-tetrachlorobenzene	36.185					F(B14)
	36.386					
1, 2, 3, 5-Cl ₄ $\emptyset$	36.816					
	36.872					
	37.020					
	37.289					
	37.483					
	37.657					
1, 2, 4, 5-tetrachlorobenzene	36.702					F(B2, B14, M7); Z(R16)
	36.738					
1, 2, 4, 5-Cl ₄ $\emptyset$	36.843					
	36.898					
Pentachlorobenzene	37.466					F(B14)
	37.504					
Cl ₅ $\emptyset$	37.720					
	37.959					
	38.153					
Hexachlorobenzene	38.381					F(B14); S(T8); T(D9, T8);
Cl ₆ $\emptyset$	38.452					Z(M23)
	38.493					

Heterocyclics and polyheterocyclics

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Chloromaleic anhydride	37.187					F(B16)
N-chlorosuccinimide	54.100					F(S7, K37)
Trichlorotriazine (Cyanuric chloride)	36.770 36.738		36.323 36.338	20°C		F(N2, B23, B21); T(D11) Z(A3, M8, M20)
2-chlorobenzothiazole	36.210					F(B16)
1, 3-dichloro-5, 5-dimethyl hydantoin	55.950 53.627					F(H8)
2, 5-dichlorothiophene	37.618 37.071					F(H8)
2-chloroethyl-chlorosulfinate	34.320					F(H8)
Tetrachloro-phthallic anhydride	38.413 38.249					F(B16)
N-chloropipidine	43.889					F(K37)

Homocyclic and Polyhomocyclic

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2,4-dichlorophenoxyacetic acid	35.146 36.226					F(B12)
2,4-Cl ₂ ϕ OCH ₂ COOH						
Para-chlorophenoxyacetic acid	34.212					F(B12)
P-Cl ϕ OCH ₂ COOH						
2,4,6-trichlorophenyl-hydrazine	35.559 35.810 36.235					F(B2)
2,4,6-Cl ₃ ϕ NHNH ₂						
Tetrachloro pthallic anhydride	38.413 38.249					F(B16)
Cl ₄ C ₆ -1,2-(CO) ₂ O						
Hexachloro cyclopentadiene	36.952 37.280 37.452 38.812 39.082					F(B16)
Hexachloro cyclohexane *	36.133					F(M10, D21)
(Gamma isomer) Lindane	36.364 36.819 36.892 37.341					
1,4-bis(trichloromethyl) benzene	38.302 38.722 38.909 39.200 39.527 39.406					F(B16)
3-chloropropenyl benzene	33.605					F(B16)

* Radiation study by D33

Homocyclics (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
1, 2, 3, 4-tetrachloro-tetrahydro-naphthalene	35.262 36.100 36.783 37.055					F(B3)
Para-chlorocinnamic acid			34.227	196°K		F(M1)
D. D. T.	34.868					F(B9)
Dichlorodiphenyltrichloroethane	34.977 38.487					
$\text{CCl}_3\text{CH}(\text{C}_6\text{H}_5\text{Cl})_2$	38.814 39.039					
Chloramine T	45.724					F(H8)
Dichloramine T	51.600					F(H8)
Tetrachlorophthallic acid	38.424 38.140					F(H8)
9, 10-dichloroanthracene	34.899					F(H8)
1-chloronaphthalene	34.606					F(H8)
4, 4'-dichlorodiphenyl sulfone	34.828					F(B12)
Phenyl-p-chlorobenzene sulfonate	35.347					F(B12)
Tetrachloronaphthalene						F(G16)
FCl_5C_6						F(K35)
Cyclopropyl chloride	34.063					F(S39)
1, 1-dichlorocyclopropane	36.610					F(S39); T(S39)
1, 1-dichloro-2, 2-dimethyl-propane	36.797					F(S39); T(S39)

Homocyclics (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2, 2, 2', 2'-tetrachloro- bicyclopropyl	37.021 37.385					F(S39); T(S39)
1, , -dichloro-2, 2-diphenyl- cyclopropane	37.242 37.353					F(S39); T(S39)
Tetrachloro naphthalene	35.238 36.768					F(G16, G20); R(G20)
Chlorocyclohexene	32.698					F(T19)
1, 1-dichlorocyclonexane	34.904 34.989					F(T19)
1, 1-dichlorocyclopentane	34.984 35.050					F(T19)

Ketones (Aliphatic)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Chloroacetone	35.075 35.484					F(A1, A2)
Sym. dichloroacetone	35.943					F(A1, A2)
Dichlorotetrafluoroacetone (sym)	37.07 37.51					F(S5)
Sym. tetrachloro-difluoro- acetone	38.652 38.845 39.064 39.275					F(S5)

Ketones (Aromatic)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-chloro-acetophenone	34.618					F(M1)
α -bromo-p-chloroacetophenone	34.822					F(B1)
α -chloro-2,4-dimethyl acetophenone			34.9	20° C		F(S4)
2,5-dichloroacetophenone	35.284 35.335					F(S4)
P-chloropropiophenone	34.702					F(B12)
4,4'-dichlorobenzophenone	35.237					F(B12)

Nitriles, isocyanates, thiazoles

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
(P-chlorophenyl) acetonitrile P-Cl ϕ CH ₂ CN	34.593 34.634					F(B12)
O-chlorobenzonitrile	35.410 35.453 35.500 35.541					F(B2)
Chloroacetonitrile CH ₂ ClCN	38.125					F(G6)
Dichloroacetonitrile CHCl ₂ CN	39.443 39.754 39.923 40.048					F(G6)
Trichloroacetonitrile CCl ₃ CN	41.553 41.666 41.730					F(G6)
O-chlorophenylcyanate O-Cl ϕ NCO	34.415					F(M1)
M-chlorophenylcyanate M-Cl ϕ NCO	34.653					F(M1)
P-chlorophenylcyanate P-Cl ϕ NCO	35.259					F(B12)
2-chlorobenzothiazole	36.219					F(B16)

Nitrobenzenes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-chloronitrobenzene	37.260					F(M1); T(D24)
M-chloronitrobenzene	35.457					F(M1); T(D24)
1-chloro-2,4-dinitrobenzene	37.796					F(W1, B3, T3, L3)
1-chloro-2,4,6-trinitrobenzene	39.367					F(B12); S(K36)
2,5-dichloronitrobenzene	35.921 37.874					F(W3); Z(N17, N25)
3,4-dichloronitrobenzene	36.488 37.055					F(W3)

Nitrogen Mustards

COMPOUND	FREQ. AT 77°	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
β -dimethylaminoethyl chloride hydrochloride	35.065				F(H8)	
γ -dimethylaninopropyl chloride hydrochloride	33.239				F(H8)	
β -diethylaminoethyl chloride hydrochloride	34.660				F(H8)	
Methyl bis (β -chloroethyl) amine hydrochloride	35.075				F(H8)	
β, β' -dichlorodiethylamine hydrochloride	35.412				F(H8)	
tri(β -chloroethyl)amine hydrochloride	35.558 35.124				F(H8)	
2-chloroethyldimethylamine	33.266				F(H8)	

Phenols

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-chlorophenol	35.37					F(S5)
M-chlorophenol	34.766 34.825					F(B12)
P-chlorophenol	34.700 34.925					F(M1); T(D24)
2-chloro-4-nitrophenol	36.175					F(B12)
4-chloro-3,5-dimethylphenol	34.348 34.415					F(B2, B12, W1)
4-chloro-3-methyl-2-nitro phenol	35.650					F(B12)
4-chloro-3-methylphenol	34.535 34.887					F(B12)
2,6-dichlorophenol	35.306* 35.819*					F(S5)
2,6-dichloro-4-nitrophenol	36.263 37.364					F(S5)
4,6-dichloro-3-methylphenol	34.749 35.540					F(B12)
2,4,6-trichlorophenol	35.262 35.400 36.770					F(B12)
Pentachlorophenol	37.129 37.375 38.192 38.579					F(B1, B12)

* two resonances

Phenols (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Hexachlorophenol	37.055 37.553 37.867 38.157 39.997 40.100					F(B3)
4-amino-2,6-dichlorophenol	35.950					F(H8)

Pyridines and pyrimidines

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2-chloropyridine	34.194					F(D8, S7)
3-chloropyridine	35.238					F(B21)
4-chloropyridine	34.739 34.748 35.031 35.042					F(B21)
5-chloro-2-aminopyridine	35.530					F(B21)
3,5-dichloropyridine	35.601					F(B21)
4,6-dichloropyridine	35.102 35.132 35.308 35.425					F(B21, B23)
2-chloropyridinium hydro- chloride	37.559					F(S7)
6-chloro-2,4-diammino- pyrimidine	34.304					F(B23)
6-chloro-2,4-dimethoxy- pyrimidine	34.618					F(B21, B23)
6-chloro-4-amino-2-methyl- mercaptopyrimidine	34.933					F(B21, B23)
2,4-dichloropyrimidine	35.310 35.321					F(B21, B22)
2,4-dichloro-5-methyl- pyrimidine	34.893 35.338					F(B23)
2,4-dichloro-6-methyl- pyrimidine	35.256					F(D11, B21, B23)

Pyridines and pyrimidines (cont.)

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2, 4-dichloro-5-ethyl-6-amino pyrimidine			34. 879 35. 044	86° K		F(D11)
4, 6-dichloro-2-methyl-5-phenyl- pyrimidine			35. 248	86° K		F(D11)
4, 6-dichloro-2-methyl- 5-benzylpyrimidine			35. 015	86° K		F(D11)
2, 4, 6-trichloropyrimidine	35. 702 36. 166 36. 250					F(D11, B23)
2, 4, 5, 6-tetrachloropyrimidine	36. 281 36. 560 37. 068 38. 020 38. 420					F(B21, B23)

Quinolines, quinones and derivatives

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2-chloroquinoline	33.271					F(S7); T(D8)
6-chloroquinoline	34.628					F(S7); T(D8)
7-chloroquinoline			34.681	86°K		F(D11)
2-chloroquinolinium hydrochloride	37.145					F(S7)
2-chloro-4-methylquinoline or 2-chloropipidine	33.665					F(B21, D11)
4,7-dichloroquinoline	34.764 35.179 35.591					F(S7)
2,4-dichloro-3-methylquinoline			34.268 35.627	86°K		F(D11)
2,5-dichloro-p-quinone	36.321					F(B21)
2,6-dichloro-p-quinone	36.266 36.361					F(B21)
2,5-dichloro-3,6-dihydroxy- p-quinone	37.148					F(B21)
2,3-dichloro-1,4-napthoquinone	37.114					F(B21)
2,3,5,6-tetrachloro-p-quinone (chloranil)	37.442 37.470 37.515 37.585					F(B12, M2, B21, D37); Z(R15)
Tetrachloro hydroquinone	37.205 37.373					F(B12)
N-chloro-p-quinoneimide	44.992					F(S7)

Quinolines (cont.)

COMPOUND	FREQ. AT 77°K	ISO. cm ⁻¹	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Chloranil-hexamethyl Benzene complex	37.504 37.716					F(D37)
1-chloroanthraquinone	37.529					F(H8)
2-chloroanthraquinone	35.390					F(H8)
1,5-dichloroanthraquinone	36.385					F(H8)
1,8-dichloroanthraquinone	36.777					F(H8)

Silanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Ethyl-trichlorosilane $C_2H_5Cl_3Si$	18.756 18.842 18.865					F(W1)
$SiCl_4$	20.467 20.415 20.408 20.273					
$SiHCl_3$	19.163 19.030 18.917					
Si_2Cl_6	19.319 19.287 19.271					
CH_3SiCl_3	19.155 19.020 18.955					
$SiHCl_2C_2H_5$	18.179 17.954					
$SiCl_2(CH_3)_2$	17.756					
$C_2H_5SiCl_2C_2H_5$	17.740 17.515					
$SiCl(CH_3)_3$	16.506					
$CH_2BrCHBrSiCl_3$	19.839 19.150					
$CH_2=CClSiCl_3$	20.361 19.401					
$CH_2=CHSiCl_3$	19.315 19.119 18.962					

Silanes (cont.)

COMPOUND	FREQ. AT 77°K or ν	ISO.	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Phenyltrichlorosilane	19.143					
1,1-dichloro-1-silocycloalkane						F(B56)
1-methyl-1-chloro- 1-silocycloalkane						F(B56)

Sulfonic Acids and Salts and Sulfinates

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2,5-dichlorobenzene sulfonic acid sodium salt $2,5\text{-Cl}_2 \text{ } \phi \text{ SO}_3\text{Na}$	35.212 36.504					F(B1)
2,5-dichlorobenzene sulfonic acid $2,5\text{-Cl}_2 \text{ } \phi \text{ SO}_3\text{H} \cdot 2\text{H}_2\text{O}$	35.622 36.160 36.450					F(B1)
2-chloro-5-nitrobenzene sulfonic acid $2\text{-Cl-5-NO}_2 \text{ } \phi \text{ SO}_3\text{H}$	36.751					F(B12)
p-chlorobenzene sulfonic acid sodium salt $p\text{-Cl } \phi \text{ SO}_3\text{Na}$	35.137					F(B1)
4-chloro-3-nitrobenzene sulfonic acid potassium $4\text{-Cl-3-NO}_2 \text{ } \phi \text{ SO}_3\text{K}$ salt	37.957					F(B2)
2-chloro-5-nitrobenzene sulfonic acid sodium salt $2\text{-Cl-5-NO}_2 \text{ } \phi \text{ SO}_3\text{Na}$	36.627					F(B2, B12)
3-chloro-4-methylbenzene sulfonic acid sodium salt $3\text{-Cl-4-CH}_3 \text{ } \phi \text{ SO}_3\text{Na}$	34.911					F(B16)
2-chloroethyl-(p-toluene) sulfonate	34.590					F(B16)
2-chloroethyl chlorosulfinate	34.320					F(H8)

Sulfonyl Chlorides

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Ethanesulfonylchloride	35.519					F(B1)
L-butan sulfonyl chloride $\text{L-CH}_3(\text{CH}_2)_3\text{SO}_2\text{Cl}$	32.759					F(B1)
Benzene sulfonyl chloride	32.470 32.538 32.892					F(M2, B1)
M-nitrobenzenesulfonylchloride	34.337					F(B3)
P-nitrobenzenesulfonylchloride	33.433					F(B3)
P-bromobenzenesulfonyl- chloride	32.895					F(B3)
P-methylbenzenesulfonyl- chloride	32.460					F(M2)
2,5-dimethylbenzenesulfonyl- chloride	32.269 32.318 32.527 32.757					F(B1)
P-chlorobenzenesulfonyl chloride	35.967					F(B3)
2,5-dichlorobenzenesulfonyl chloride	34.448 36.391 37.320					F(B1)
2-thiophenesulfonylchloride	33.151					F(B1)

Tolunes, Xylenes

COMPOUND	FREQ.	ISO.	FREQ.	TEMP.	COUPLING CONSTANT	REFERENCES
α -chlorotoluene	33.630					F(M1, L1)
α, α, α -trichlorotoluene	38.288 38.702 38.713 38.786 38.824 38.898					F(M2)
α -chloro-p-chlorotoluene	34.507 33.754					F(B2, M1); Z(M9)
α -chloro-p-nitrotoluene	34.311					F(B3, B22)
O-chlorobenzyltrifluoride	35.633					F(M1)
M-chlorobenzyltrifluoride	35.073					F(B16)
2-chloro-6-nitrotoluene	35.219					F(B12)
2,4-dichlorobenzylchloride	35.505					F(B16)
P-fluoro- α, α, α -trichloro- toluene	38.772 39.056					F(M2)
α -chloro-m-nitrotoluene	34.216					F(H8)
α, α' -dichloro-p-xylene	33.863					F(H8)
$\alpha, 0$ -dichlorotoluene	35.225 34.560 34.795					F(H8)
$\alpha, 3, 4$ -trichlorotoluene	36.232 36.436 35.854 35.673					F(H8)
2,6-dichlorotoluene	34.788 34.755					F(H8)

Acetanilides

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-bromoacetanilide P-Br ϕ NHCOCH ₃	226.805	Br ⁸¹				F(B5, B8)
4-bromo-2-methylacetanilide	225.47	Br ⁸¹				F(H8)
2-bromo-4-methylacetanilide	229.93	Br ⁸¹				F(H8)

Aliphatic Acids and Derivatives

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Bromoacetic acid CH_2BrCOOH	286.74 284.55	Br^{79}				F(B4, B6, B8, S3)
2-bromoethylacetate	261.785	Br^{79}				F(H8)
β -propionic acid	259.997	Br^{79}				F(H8)
2-bromoethylamine hydro- bromide	263.874	Br^{79}				F(H8)

Alkyl Bromomethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
CH_3Br	220.931	Br^{81}				F(D16, R1, D25, Z1, K1, H1, D36)
CH_2Br_2	234.805 235.601	Br^{81}				F(H1, Z1, R1, D36)
CHBr_3	250.527 250.666 251.970	Br^{81}				F(K3, Z1, D36, B28, R1)
CBr_4	268.0*	Br^{81}				F(H1, S1)
CF_3Br	252.263	Br^{81}				F(Z1, R1)
CF_2Br_2	251.624 255.681	Br^{81}				F(Z1)
CFBr_3	255.592 262.371	Br^{81}				F(Z1)
CD_3Br	220.563					F(D25)

* six lines

Alkyl, Bromoethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
1, 2-dibromoethane	216.827 218.977	Br ⁸¹				F(K1, Z1, S3, D36); T(D32)
Bromoethane	207.790	Br ⁸¹				F(H1, Z1, K3, D36)
Sym tetrabromoethane	249*	Br ⁷⁹				F(S4)

* six lines

Alkyl, Bromopropanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Bromopropane	210.277	Br ⁸¹				F(K3, Z1, D36)
1, 3-dibromopropane	249.822 251.820 252.591	Br ⁷⁹				F(S4)
1, 2, 3-tribromopropane	265.040 268.653 269.685	Br ⁷⁹				F(S4)

2

Alkyl, Bromo-anes (higher than propanes)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
N-butyl bromide		Br ⁸¹	208.86	83°K		F(K3)
1-bromohexane	249.358	Br ⁷⁹				F(S4)
Bromcyclohexane	242.108	Br ⁷⁹				F(S4)
N-octylbromide	249.434	Br ⁷⁹				F(S4)
1-bromoheptane	208.343	Br ⁸¹				F(H8)
1, 3-dibromobutane	209.771	Br ⁸¹				F(H8)
1, 5-dibromopentane	212.512	Br ⁸¹				F(H8)

Anilines

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-bromoaniline	220.255	Br ⁸¹				F(B5, B8)
M-bromoaniline	222.614	Br ⁸¹				F(B5, B8, L4)
P-bromoaniline	221.862	Br ⁸¹				F(B5, B6, B8, A4, H1, L4)
P-bromoaniline hydrochloride	232.043	Br ⁸¹				F(B8)
P-bromo-N, N-dimethylaniline		Br ⁷⁹	254.20 255.10 256.03	25° C		F(L4)
P-bromo-N, N-diethylaniline	263.444 262.906	Br ⁷⁹				F(B4)
2-bromo-4-methyl aniline	265.974 263.222	Br ⁷⁹				F(B4)
4-bromo-2-methyl aniline	263.616	Br ⁷⁹				F(B5)
2, 4, 6-tribromoaniline	230.095 230.752 233.563	Br ⁸¹				F(B5, B8, L4, M6)
2, 6-dibromo-4-nitroaniline	282.458	Br ⁷⁹				F(S36)

Anisoles, Phenetoles

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-bromoanisole	233.250	Br ⁸¹				F(B5, B8)
P-bromoanisole	226.690	Br ⁸¹				F(B5, B8)
2, 4, 6-tribromoanisole	280.632 283.888 289.194	Br ⁷⁹				F(B5, L4)
P-bromophenetole	266.813	Br ⁷⁹				F(B4)
β -bromophenetole	262.548	Br ⁷⁹				F(H8)

Benzoic Acids and Derivatives

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-bromobenzoic acid	234.185	Br ⁸¹				F(B6, B8, L4)
M-bromobenzoic acid	226.434	Br ⁸¹				F(L4)
P-bromobenzoic acid		Br ⁷⁹	280.08	20° C		F(L4)
2-bromo-3-nitrobenzoic acid		Br ⁷⁹	302.54	20° C		F(L4)
4-bromo-2-hydroxybenzoic acid (4-bromosalicylic acid)	271.820	Br ⁷⁹				F(B5)
M-bromo-methylbenzoate	271.772	Br ⁷⁹				F(B5)
P-bromo-methylbenzoate	275.960	Br ⁷⁹				F(B5)
5-bromo-2-hydroxy benzoic acid	227.08	Br ⁸¹				F(H8)

Bromobenzenes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONTRAST	REFERENCES
Bromobenzene	268.856	Br ⁷⁹				F(A4, B5, C6, H1, L4)
O-dibromobenzene	236.068	Br ⁸¹				F(C6)
P-dibromobenzene*	226.49	Br ⁸¹				F(H1, B5, C6, L4, S1, M6); P(F1); R(G5); S(D22); T(D17, F1); Z(D17, K19, S16)
1, 2, 4-tribromobenzene	277.985 282.940 286.650 288.080	Br ⁷⁹				F(B5, C6)
1, 3, 5-tribromobenzene	279.075 280.228 280.721	Br ⁷⁹				F(B5, C6, H1, L4)
1, 2, 3, 5-tetrabromobenzene	236.042 242.176 242.767 244.949 246.140 249.314	Br ⁸¹				F(C6)
1, 2, 4, 5-tetrabromobenzene	289.675 290.572	Br ⁷⁹				F(B5, C6)
Hexabromobenzene	305.922 305.332 305.235	Br ⁷⁹				F(C6)

* Radiation study by D43

Carbonyl Bromides

COMPOUND	FREQ. AT 77°K or ν	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Acetyl bromide	178.082 179.536 180.140 181.350	Br ⁸¹				F(B4)
Bromoacetyl bromide	234.87 244.34	Br ⁷⁹				F(S4)
Benzoyl bromide	191.868	Br ⁸¹				F(B4)
M-bromobenzoyl chloride	277.360	Br ⁷⁹				F(S4)

Homocyclics, Multicyclics and Heterocyclics

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-bromosulfonyl chloride	236.665 236.642	Br ⁸¹				F(B6, B8)
α -bromo-1,4-dimethylbenzene	263.332 254.290	Br ⁷⁹				F(B4, B5)
Bromocyclohexane	242.108	Br ⁷⁹				F(S4)
P-bromophenyl-phenylether	272.500	Br ⁷⁹				F(B4)
4,4'-dibromobiphenyl	267.439 269.461 271.110 271.835	Br ⁷⁹				F(A1, B5)
1-bromonaphthalene	267.394	Br ⁷⁹				F(B4)
9,10-dibromoanthracene	272.975 275.053	Br ⁷⁹				F(B5, L4)
P-bromodiphenyl		Br ⁷⁹	268.70	20° C		F(L4)
Sym. tribromophenyl-p- toluenesulfonate		Br ⁷⁹	281.12 288.40 297.06			F(L4)
1-bromo-4-fluorobenzene	228.14	Br ⁸¹				F(H8)
2-bromo-1,4-dimethylbenzene	219.99	Br ⁸¹				F(H8)
2,5-dibromotoluene	226.51 228.29	Br ⁸¹				F(H8)
2,4,6-tribromophenyl-p- toluenesulfonate	239.438 244.424 250.744	Br ⁸¹				F(H8)
1,2,3,4,5,6-hexabromo- cyclohexane	237.645 239.477 241.396	Br ⁸¹				

Homocyclics (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-bromophenylhydrazine · HCl	280.131	Br ⁷⁹				F(H8)
Bis(p-bromophenyl)ether	278.461	Br ⁷⁹				F(H8)
β -bromostyrene	268.043 267.364	Br ⁷⁹				F(H8)
α -3-camphor	270.564	Br ⁷⁹				F(H8)
3-bromotropolene	232.05	Br ⁸¹				F(I11)
4-bromotropolene	226.96	Br ⁸¹				F(I11)
5-bromotropolene	226.15	Br ⁸¹				F(I11)
3,5-dibromotropolene	233.17 240.86	Br ⁸¹				F(I11)
3,7-dibromotropolene	237.21 237.86	Br ⁸¹				F(I11)
3,5,7-tribromotropolene	241.40	Br ⁸¹				F(I11)
α, α' -dibromoparaxylene	257.647	Br ⁷⁹				F(S36)
Monofluoro-pentabromo benzene	305.61 305.99 307.20 309.30 309.72	Br ⁷⁹				F(S36, K35)

Homocyclics (cont.)

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Bromocyclopentane	244.15					F(T19)
Trans, 1, 4-dibromocyclo- hexane	248.071 248.182					F(T18, T19); T(T18)
Cis, 1, 4-dibromocyclohexane	245.125 246.296					F(T18, T19); T(T18)
Trans, 3, 5-dibromocyclopenta- diene	248.538 251.920					F(T19)
N-bromoacetamide	344.1					F(K37)
N-bromo-2-pyrrolidinone	343.3					F(K37)
N-bromo- ϵ -caprolactam	341.9					F(K37)
N-bromosuccinimide	358.73					F(K37)
N-bromophthalimide	370.8					F(K37)

Ketones

COMPOUND	FREQ. AT 77°K	ISO. $\sigma = \nu$	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-bromoacetophenone	230.670 231.107	Br ⁸¹				F(B5, B6, B8)
α -bromoacetophenone	230.656	Br ⁸¹				F(B6)
P-chloro- α -bromoacetophenone	233.162	Br ⁸¹				F(B8)
α -bromobenzal acetophenone $C_6H_5CH:C(Br)COC_6H_5$		Br ⁷⁹	276.30	20° C		F(L4)

Nitrobenzenes

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-bromonitrobenzene	247.486	Br ⁸¹				F(H1, L4)
M-bromonitrobenzene	233.630	Br ⁸¹				F(L4, H1)
P-bromonitrobenzene	232.568	Br ⁸¹				F(L4, H1)
1, bromo-2, 4-dinitrobenzene	301.270	Br ⁷⁹				F(B5)
2, 5-dibromonitrobenzene	287.2 307.1	Br ⁷⁹				F(H1)

Phenols

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-bromophenol	275.884	Br ⁷⁹				F(B4, L4)
M-bromophenol	271.420 272.745	Br ⁷⁹				F(B4, L4,
P-bromophenol	268.222 269.683 271.500 274.795	Br ⁷⁹				F(A4, B5, H1, L4)
2,4-dibromophenol	228.933 230.429 230.300 231.657 232.303 234.654	Br ⁸¹				F(S4)
2,6-dibromophenol		Br ⁸¹	228.176	20° C		F(S4)
2,6-dibromo-4-amino-phenol		Br ⁷⁹	274.79 277.80	20° C		F(L4)
2,6-dibromo-4-nitro-phenol	283.931 284.569 298.553	Br ⁷⁹				F(L4)
Sodium 2,6-dibromo-4-nitro-phenolate		Br ⁷⁹	270.32 270.71	20° C		F(L4)
1,6-dibromo-2-naphthol		Br ⁷⁹	265.15 267.87	20° C		F(L4)
2,4,6-tribromophenol		Br ⁷⁹	275.96 277.17 284.40	20° C		F(L4)
Pentabromophenol	246.370 251.05 255.01	Br ⁸¹				F(H8)

Pyridines, pyrimidines

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2-bromopyridine	265.213	Br ⁷⁹			F(S7)	
3, 5-dibromopyridine	278.005	Br ⁷⁹			F(S7)	

Quinones, Quinolines

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
3-bromoquinoline	278.005	Br ⁷⁹				F(S7)
2,6-dibromo-N-chloro-p- quinoneimide	246.736	Br ⁸¹				F(S7)
Tetrabromo-p-quinone	298.100 298.974	Br ⁷⁹				F(S36)

Alkyl,Iodomethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Cl_4	319.549	1			2130.33	F(R1, D36)
$\text{CHI}_3 \cdot 3\text{S}_i$	307.106 613.949	1 2			2046.634	F(R1, D36)
CH_2I_2	286.883 568.362	1 2			1897.368	F(R1, H1, Z1, D36)
CH_3I	265.102 529.670	1 2			1765.846	F(A4, D2, H1, K4, R1, S22, Z1, D26); S(K22)
CD_3I	264.591	1				F(D25)
CF_3I		1	310.375	83°K	2069.17	F(R1, S22)

Alkyl Iodethanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Iodoethane		1	247.115	83°K		F(Z1, H1, K4, D36)
		1	247.374			
		2	494.058			
		2	-----			
Acetylene di-iodide(trans) CHICI		1	277.1	83°K	1847.0	F(D2); S(K22)

Alkyl Iodopropanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
1-Iodopropane		1	250.810	83°K		F(Z1, K4, D36)
		1	250.962			
		2	499.810			
		2	-----			
2-iodopropane	238.946	1				F(S4, Z1, D36)

Alkyl Iodoanes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
N-butyl iodide		1	249.062	83°K		F(K4)
		2	497.539			

Anilines

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-iodoaniline	267.381	1				F(L4, H1)
M-iodoaniline	270.491	1				F(S4)
P-iodoaniline	264.307	1				F(H1, L4, S36)
P-iodoaniline hydrochloride		1	288.28	20° C	1909.5	F(L4)
		2	546.06			

Anisoles, phenetoles

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-iodoanisole	287.216	1				F(B16)
M-iodoanisole	274.593	1				F(B16)

Benzoic Acids and Esters

COMPOUND	FREQ. AT 77° K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-iodobenzoic acid	297.791	1			1919.6	F(B6, L4)
	573.43	2				
M-iodobenzoic acid	278.570	1			1830.0	F(B6, H1, L4)
	548.56	2				
P-iodobenzoic acid		1	272.89	25° C	1814.8	F(L4)
		2	544.18			
Sodium o-iodobenzoate		1	294.81	25° C		F(L4)
Sodium m-iodobenzoate		1	272.73	25° C		F(L4)
		1	273.76		1817.4	
		2	545.17		1824.8	
		2	547.12			
Sodium p-iodobenzoate		1	277.59	25° C		F(L4)
		1	280.82			
		1	282.25			
Methyl m-iodobenzoate		1	276.24	25° C	1835.0	F(L4)
		2	550.16			
Methyl p-iodobenzoate		1	284.03	25° C	1882.7	F(L4)
		2	564.21			
3,5-diiodo-2-hydroxy benzoic acid		1	284.19	25° C		F(L4)
		1	295.14			

Homocyclics, heterocyclics, Aliphatics

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
P-iodacetanilide	277.883	1			1820.9	F(H1, L4)
Iodoacetic acid		1	297.86	83°K		F(K4)
		1	298.37			
		2	592.79			
		2	596.12			
β -iodopropionic acid		1	260.9	90°K		F(A4)
Tetraiodo-phthallic anhydride		1	313.63	28° C		F(L4)
		1	316.20			
		1	324.03			
		1	328.33			
4-iodobiphenyl		1	275.40	25° C		F(L4)

Iodobenzenes						
COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
Iodobenzene	274.530	1			1834.7	F(H1, L4, S36)
	275.024	1			1839.4	
M-diiodobenzene		1	280.3	20° C		F(H1, L4)
P-diiodobenzene		1	275.89	28° C	1834.7	F(H1, S1, L4, S36)
		1	276.31		1839.4	
		2	550.16			
		2	551.68			
Iodoxybenzene $\text{O}_2\text{IC}_6\text{H}_5$		1	-----	21° C		F(L4)
		1	162.23		-----	
		2	293.30		1045.9	
		2	311.70			

Nitrobenzenes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-iodonitrobenzene		1	315.19	20° C		F(L4)
		1	315.97		2055.0	
		2	613.38		2059.9	
		2	615.26			
M-iodonitrobenzene		1	285.63	20° C		F(L4, B6, A4)
		1	286.66		1901.5	
		2	570.29		1905.8	
		2	571.43			
P-iodonitrobenzene		1	284.36	20° C		F(L4)
		2	565.82		1887.7	

Phenols

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
O-iodophenol		1	277.60	20° C		F(L4)
		2	551.80		1841.1	
M-iodophenol		1	272.1	20° C		F(H1, L4)

Toluenes, Xylenes

COMPOUND	FREQ. AT 77°K	ISO. or ν	FREQ. AT T°	TEMP.	COUPLING CONSTANT	REFERENCES
2-iodo-paraxylene	270.770	1				F(S4)
2-iodo-metaxylene	273.353	1				F(S4)
2,5-diiodo- α, α, α -trifluoro- toluene		1	287.2	20° C		F(H1)

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JOURNAL ABBREVIATIONS USED

AC	Acta Crystallographica
BAPS	Bulletin of the American Physical Society
BCJS	Bulletin of the Chemical Society of Japan
CJP	Canadian Journal of Physics
CR	Comptes Rendus
CS	Current Science
FTT	Fizika Tverdogo Tela
HPA	Helvetica Physica Acta
IRE	Institute of Radio Engineers
JACS	Journal of the American Chemical Society
JAP	Journal of Applied Physics
JCP	Journal of Chemical Physics
JCSL	Journal of the Chemical Society (London)
JIC	Journal of Inorganic Chemistry
JPC	Journal of Physical Chemistry
JPCS	Journal of the Physics and Chemistry of Solids
JPSJ	Journal of the Physical Society of Japan
OS	Optics and Spectroscopy
P	Physica
PL	Physics Letters
PPSL	Proceedings of the Physical Society (London)
PR	Physical Review
PRL	Physical Review Letters

R-26

SPSS	Soviet Physics -- Solid State
T	Tetrahedron
TCA	Theoretica Chimica Acta
ZN	Zeitschrift für Naturforschung
ZP	Zeitschrift für Physik
ZSK	Zhurnal Strukturnoi Khimii