

Infrared Characteristic Group Frequencies

Tables and Charts

Second Edition

GEORGE SOCRATES

Brunel, The University of West London, Middlesex, United Kingdom

JOHN WILEY & SONS

Chichester · New York · Brisbane · Toronto

Contents

List of Charts and Figures	ix		
Preface to the First Edition	x		
Preface to the Second Edition	xiii		
Symbols Used	xiv		
1 Introduction	1		
Spurious Bands in Infrared Spectra	2		
Spurious Bands at Any Position	3		
Spurious Bands at Specific Positions	6		
Positive and Negative Spectral Interpretation	8		
Negative Spectral Interpretation	8		
Positive Spectral Interpretation	8		
Regions for Preliminary Investigation	8		
Preliminary Regions to Examine	8		
Confirmation	9		
Chemical Modification	30		
Collections of Reference Spectra	30		
References	32		
2 Alkane Group Residues: C—H Group	34		
Alkane Functional Groups	34		
Alkane C—H Stretching Vibrations	34		
Alkane C—H Deformation Vibrations	34		
Alkane C—C Vibrations: Skeletal Vibrations	35		
References	41		
3 Alkenes, Oximes, Imines, Amidines, Azo Compounds: C=C, C=N, N=N Groups	42		
Alkene Functional Group, $\diagup\text{C}=\text{C}\diagdown$	42		
Alkene C=C Stretching Vibrations	42		
Alkene C—H Stretching Vibrations	42		
Alkene C—H Deformation Vibrations	42		
Alkene Skeletal Vibrations	43		
Oximes, Imines, Amidines etc.	50		
Azo Compounds, —N=N—	50		
References	51		
4 Triple-bond Compounds: —C≡C—, —C≡N, —N≡C, —N≡N Groups	52		
Alkyne Functional Group, —C≡C—	52		
Alkyne C≡C Stretching Vibrations	52		
Alkyne C—H Vibrations	52		
Alkyne skeletal Vibrations	52		
Nitriles, —C≡N	54		
Isonitriles, —N≡C	54		
Nitrile <i>N</i> -Oxides, —C≡N → O	54		
Cyanamides, $\diagup\text{N}-\text{C}\equiv\text{N}$	54		
Diazonium Salts, Aryl—N≡N ⁺ X ⁻	56		
References	56		
5 Cumulated Double-bond Compounds: X=Y=Z Group	57		
Allenes, $\diagup\text{C}=\text{C}=\text{C}\diagdown$	57		
Isocyanates, —N=C=O and Cyanates	57		
Isothiocyanates, —N=C=S	58		

Thiocyanates, $-\text{S}-\text{C}\equiv\text{N}$	58	10 The Carbonyl Group: $\text{C}=\text{O}$	80
Selenocyanates and Isoselenocyanates	58	Introduction	80
Azides, $-\text{N}=\text{N}^+=\text{N}^-$	59	Ketones, $\text{>C}=\text{O}$	80
Diazo Compounds, $\text{>C}=\text{N}^+=\text{N}^-$	61	Ketone $\text{C}=\text{O}$ Stretching Vibrations	84
Carbodi-imides, $-\text{N}=\text{C}=\text{N}-$	61	Methyl and Methylene Deformation Vibrations in Ketones	85
References	61	Ketone Skeletal and Other Vibrations	85
		Quinones	87
6 Hydroxyl Group Compounds: $\text{O}-\text{H}$ Group	62	Aldehydes, $-\text{CHO}$	88
Alcohols, $\text{R}-\text{OH}$	62	Aldehyde $\text{C}=\text{O}$ Stretching Vibrations	88
Alcohol $\text{O}-\text{H}$ Stretching Vibrations	62	Aldehydic $\text{C}-\text{H}$ Vibrations	88
Alcohol $\text{C}-\text{O}$ Stretching Vibrations	62	Other Aldehyde Bands	89
Alcohol $\text{O}-\text{H}$ Deformation Vibrations	62	Carboxylic Acids, $-\text{COOH}$	90
Phenols	66	Carboxylic Acid $\text{O}-\text{H}$ Stretching Vibrations	90
Cellulose and its Derivatives	66	Carboxylic Acid $\text{C}=\text{O}$ Stretching Vibrations	90
References	67	Other Vibrations of Carboxylic Acids	90
		Carboxylic Acid Salts	91
7 Ethers: $\text{G}^1-\text{O}-\text{G}^2$	68	Carboxylic Acid Anhydrides, $-\text{CO}-\text{O}-\text{CO}-$	93
References	71	Carboxylic Acid Halides $-\text{CO}-\text{X}$	94
		Diacyl Peroxides, $\text{R}-\text{CO}-\text{O}-\text{O}-\text{CO}-\text{R}$ (acid peroxides), and Peroxy Acids, $-\text{CO}-\text{OOH}$	95
8 Peroxides and Hydroperoxides: $-\text{O}-\text{O}-$ Group	72	Esters, $-\text{CO}-\text{O}-$ Carbonates, $-\text{O}-\text{CO}-\text{O}-$ and Chloroformates, $-\text{O}-\text{CO}-\text{Cl}$	96
References	73	Ester $\text{C}=\text{O}$ Stretching Vibrations	96
		Ester $\text{C}-\text{O}-\text{C}$ Stretching Vibrations	97
9 Amines, Imines, and Their Hydrohalides	74	Other Ester Bands	97
Amine Functional Groups	74	Lactones	103
Amine $\text{N}-\text{H}$ Stretching Vibrations	74	Amides, $-\text{CO}-\text{N}<$	104
Amine $\text{N}-\text{H}$ Deformation Vibrations	74	Amide $\text{N}-\text{H}$ Stretching Vibrations	104
Amine $\text{C}-\text{N}$ Stretching Vibrations	74	Amide $\text{C}=\text{O}$ Stretching Vibrations: Amide I Band	105
Amine $\text{>N}-\text{CH}_3$ and $\text{>N}-\text{CH}_2-$ Absorptions	75	Amides $\text{N}-\text{H}$ Deformation and $\text{C}-\text{N}$ Stretching Vibrations: Amide II Band	105
Other Amine Bands	75	Other Amide Bands	105
Amine Hydrohalides, $-\text{NH}_3^+$, >NH_2^+ , >NH^+ and Imine	75	Hydroxamic Acids, $-\text{CO}-\text{NHOH}$	106
Hydrohalides, $\text{>C}=\text{NH}^+-$	75	Hydrazides, $-\text{CO}-\text{NH}-\text{NH}_2$ and $-\text{CO}-\text{NH}-\text{NH}-\text{CO}-$	109
Amine Hydrohalide $\text{N}-\text{H}^+$ Stretching Vibrations	75	Lactams (Cyclic Amides)	110
Amine Hydrohalide $\text{N}-\text{H}^+$ Deformation Vibrations	75	Imides, $-\text{CO}-\text{NH}-\text{CO}-$	111
Amine and Imine Hydrohalides: Other Bands	75	Ureas, $\text{>N}-\text{CO}-\text{N}$ (Carbamides)	113
References	79	Urethanes, $\text{>N}-\text{CO}-\text{O}-$ (Carbamates)	113
		Amino Acids	115
		Free Amino Acid $-\text{NH}_3^+$ Vibrations	115

Free Amino Acid Carboxyl Bands	115	13 Five-membered Ring Heterocyclic Compounds	140
Amino Acid Hydrohalides	116	Pyrroles and Indoles	140
Amino Acid Salts	116	Pyrrolines	140
Amido Acids, $\begin{array}{c} \diagup \\ \text{N} \\ \diagdown \end{array} \text{—CO—}\cdots\text{COOH}$	117	Furans	142
Proteins and Peptides	117	Thiophenes	144
References	118	Imidazoles	145
		Pyrazoles	146
		References	147
11 Aromatic Compounds	121	14 Organic Nitrogen Compounds	148
Aromatic C—H Stretching Vibrations	122	Nitro Compounds, —NO_2	148
Aromatic In-plane C—H Deformation Vibrations	122	Nitroso Compounds (and Oximes)	150
Aromatic Out-of-plane C—H Deformation Vibrations and Ring		Covalent Nitrates	152
Out-of-plane Vibrations in the Region $900\text{--}650\text{ cm}^{-1}$	122	Nitrites	152
Aromatic C=C Stretching Vibrations	123	References	154
Overtone and Combination Bands	123		
Aromatic Ring Deformation Vibrations below 700 cm^{-1}	125	15 Organic Halogen Compounds	155
Polynuclear Aromatic Compounds	127	Organic Halogen Compounds, $\begin{array}{c} \diagup \\ \text{C} \\ \diagdown \end{array} \text{—X}$	155
Naphthalenes	127	Organic Fluorine Compounds	155
Anthracenes and Phenanthrenes	127	Organic Chlorine Compounds	155
References	128	Organic Bromine Compounds	156
		Organic Iodine Compounds	156
		Aromatic Halogen Compounds	156
		References	160
12 Six-membered Ring Heterocyclic Compounds	130	16 Sulphur and Selenium Compounds	161
Pyridine Derivatives	130	Mercaptans, —SH	161
Aromatic C—H Stretching Vibrations	130	C—S and S—S Vibrations: Organic Sulphides, $\begin{array}{c} \diagup \\ \text{S} \\ \diagdown \end{array}$, Mercaptans,	
Overtone and Combination Bands	130	—SH , Disulphides, —S—S— , and Polysulphides, $(\text{—S—S—})_n$	161
C=C and C=N Stretching Vibrations	130	Compounds Containing S=O: Organic Sulphoxides, $\begin{array}{c} \diagup \\ \text{S}=\text{O} \\ \diagdown \end{array}$, and	
Ring C—H Deformation Vibrations	131	Sulphites, —O—SO—O—	164
Other Bands	131	Organic Sulphones, $\begin{array}{c} \diagup \\ \text{SO}_2 \\ \diagdown \end{array}$	166
Pyridine N-Oxides	131	Sulphonyl Halides, $\text{—SO}_2\text{—X}$	167
Other Comments	131	Sulphonamides, $\text{—SO}_2\text{—N} \begin{array}{c} \diagdown \\ \diagup \end{array}$	167
Quinolines and Isoquinolines	133	Covalent Sulphonates, $\text{R—SO}_2\text{—OR}'$	168
Pyrimidines	133		
Quinazolines	134		
Purines	135		
Phenazines	136		
Sym-triazines	136		
Melamines	137		
References	139		

Organic Sulphates, $-\text{O}-\text{SO}_2-\text{O}-$	168	Nitrogen-Hydrogen Groups	205
Sulphonic Acids, $-\text{SO}_3\text{H}$, and Salts, SO_3^-M^+	168	References	205
Thiocarbonyl compounds, $\text{>C}=\text{S}$	170		
Reviews	173	21 Inorganic Compounds and Coordination Complexes	206
Organic Selenium Compounds	173	Ions	219
Seneloamides, $\text{>N}-\text{CSe}-$	173	Coordination Complexes	219
The $\text{Se}=\text{O}$ Stretching Vibration	173	Isotopic Substitution	220
The $\text{P}=\text{Se}$ Stretching Vibration	173	Coordination of Free Ions having Tetrahedral Symmetry	220
References	176	Coordination of Free Ions having Trigonal-planar Symmetry	221
		Coordination of Free ions having Pyramidal Structure	221
		Coordinate Bond Vibration Modes	222
		Structural Isomerism	222
17 Organic Phosphorus Compounds	177	<i>Cis-Trans</i> Isomerism	222
P-H and P-C Vibrations	177	Lattice Water and Aquo Complexes	222
P-OH and P-O Vibrations	177	Metal-Alkyl Compounds	222
P-O-C Vibrations	177	Metal Halides	223
P=O Vibrations	177	Metal- π -Bond and Metal- σ -bond Complexes—Alkenes,	
Other Bands	178	Alkynes, etc.	227
References	187	Alkenes	228
		Alkynes	229
		Cyclopentadienes	229
18 Organic Silicon Compounds	188	Metal-Cyano and Nitrile Complexes	232
Si-H Vibrations	188	Ammine, Amido, Urea and Related Complexes	233
Methyl-Silicon Compounds, $\text{Si}-\text{CH}_3$	188	Metal Carbonyl Compounds	233
Ethyl-Silicon Compounds	188	Metal-Acetylacetonato Compounds, Carboxylate Complexes	
Alkyl-Silicon Compounds	189	and Complexes Involving the Carbonyl Group	235
Aryl-Silicon Compounds	189	Carboxylate Complexes and other Complexes Involving the Carbonyl	
Si-O Vibrations	189	Group	236
Silicon-Nitrogen Compounds	189	Metal Oxides and Other Inorganic Oxides	237
Silicon-Halide Compounds	189	Nitro- ($-\text{NO}_2$) and Nitrito- ($-\text{ONO}$) Complexes	237
Hydroxyl-Silicon Compounds	190	Thiocyanato ($-\text{SCN}$) and Isothiocyanato ($-\text{NCS}$) Complexes	238
References	194	Isocyanates, $\text{M}-\text{NCO}$	240
		Hydrides	240
19 Boron Compounds	195	Nitrosyl Complexes	242
References	201	Azides, $\text{M}-\text{N}_3$ and Dinitrogen and Dioxygen Complexes	242
		References	243
20 The Near Infrared Region	202	Appendix Further Reading	245
Carbon-Hydrogen Groups	202		
Oxygen-Hydrogen Groups	204		
Carbonyl Groups	204	Index	246