

Contents

Preface	xv
Acknowledgment	xvii
1 Introduction	1
1-1. Principles and Selection Rules	1
1-2. Characteristic Frequencies	4
1-3. The Need to Re-examine the IR and Raman Characteristic Frequencies	
References	7
2. Alkanes	9
2-1. Acyclic Alkanes	9
2-2. Cycloalkanes .	19
References	
3. Halocompounds	29
3-1. Monohaloalkanes	29
3-2. Effect of Other Substituents	34
3-3. Dihalogenated and Polyhalogenated Alkanes	35
3-4. Cycloalkyl Halides	37
3-5. Halogenated Alkenes and Ethynes	39
3-6. Fluorocompounds	40
3-7. Aryl Halides	41
References	42

4. Alcohols and Phenols	45
4-1. Introduction	45
4-2. O—H Stretching	45
4-3. O—H Bending	56
4-4. Skeletal Vibrations	57
References	59
5. Ethers and Peroxides	61
5-1. Introduction	61
5-2. Aliphatic Ethers	63
5-3. Acetals	65
5-4. Vinyl Ethers	65
5-5. Aromatic Ethers	65
5-6. Epoxy Compounds	68
5-7. Peroxides	68
5-8. CH Vibrations in O—CH ₃ and O—CH ₂ Groups	71
References	71
6. Alkenes	73
6-1. Alkyl-Substituted Ethylenes	73
6-2. C=C Stretching	73
6-3. Cyclic C=C Stretching	76
6-4. Olefinic C—H Stretchings	77
6-5. Olefinic C—H Out-of-Plane Deformations	78
6-6. Olefinic C—H In-Plane Deformations	82
6-7. Skeletal Vibrations	82
6-8. The Symmetric CH ₃ Deformation of C=C—CH ₃ Groups	83
6-9. Allyl Compounds	83
6-10. Other Substituted Ethylenes	84
6-11. Conjugation with a C=C Moiety	86
6-12. Conjugation with a C=O Moiety (α, β -Unsaturated Carbonyl Moieties)	88
6-13. Conjugation with a Phenyl Group	90
6-14. Conjugation with a Nitrile (C≡N) Group	91
References	

7. Acetylenes	95
7-1. Introduction	95
7-2. The C—H Stretching of C≡C—H Groups	96
7-3. The C—H Bendings of C≡C—H Groups	99
7-4. C≡C Stretching	101
7-5. The C—C Stretching of C≡C—C Moieties	102
7-6. ≡C—C Bendings	103
References	103
8. The —C≡N and N≡C Groups	
8-1. Introduction	105
8-2. Nitrile Compounds (C—CN)	107
8-3. Cyanamides (>N—C≡N)	111
8-4. Cyanates, Thiocyanates, and Selenocyanates	112
8-5. Isocyanides (C—N≡C)	113
References	113
9. Compounds Containing the Carbonyl Group	117
9-1. Introduction	117
9-2. Factors That Shift Carbonyl Bands	118
9-3. Aldehydes (—CH(=O))	122
9-4. Ketones	127
9-5. Esters	134
9-6. Carboxylic Acids	137
9-7. Anhydrides	142
9-8. Amides, Lactams, Ureas, and Imides	143
9-9. Aliphatic Acid Halides	146
9-10. Aromatic Acid Halides	149
References	151
10. Compounds Containing NH₂, NHR, and —NR₂ Groups	
10-1. Introduction	155
10-2. NH ₂ Stretching	160
10-3. NH ₂ Scissors Deformation	162
10-4. NH ₂ Wagging Mode	163
10-5. N—H Stretching	164
10-6. C—N—H Bending	166
10-7. N—H Wagging	167

10-8. Skeletal Vibrations	167
10-9. Skeletal Vibrations	170
10-10. The N—CH ₂ — and N—CH ₃ Groups	171
10-11. Amine Salts	172
10-12. Hydroxylamines (—O—NH ₂) and Hydrazines (>N—N<)	174
References	175
11. The Nitro Group	
11-1. NO ₂ Stretchings	179
11-2. C—N Stretching	185
11-3. NO ₂ Deformations	186
11-4. Covalent Nitrates (—O—NO ₂)	187
11-5. Nitroamines (>N—NO ₂)	187
References	188
12. Double Bonds Containing Nitrogen Atoms	
12-1. C-Nitroso Compounds	191
12-2. Nitrosoamines (>N—N=O)	194
12-3. Nitrites (—O—N=O)	195
12-4. Azo Compounds (—N=N—)	196
12-5. Azoxy Compounds (—N=N(→O)—)	199
12-6. Azothio Compounds (—N=N(→S)—)	199
12-7. Compounds Containing the C=N Group	199
12-8. Compounds Containing the N=S Group	209
References	209
13. Cumulated Double Bonds	
13-1. Introduction	213
13-2. Allenes (>C=C=C<)	214
13-3. Ketenes (>C=C=O)	215
13-4. Ketene Imines (>C=C=N—)	217
13-5. Diazo Compounds (>C=N=N)	218
13-6. Isocyanates (—N=C=O)	218
13-7. Isothiocyanates (—N=C=S)	219
13-8. Isoselenocyanates (—N=C=Se)	220
13-9. Azides (—N=N=N)	221
13-10. Carbodiimides (—N=C=N—)	221
References	222

14. Organic Sulfur Compounds

14-1. Introduction	225
14-2. Thiols (R-SH and Ar-SH)	225
14-3. Sulfides (Y-S-Y'; Y, Y' = R and/or Ar)	228
14-4. Disulfides (Y-S-S-Y'; Y, Y' = R and/or Ar) and Polysulfides	231
14-5. Thiocarboxylic Acids and Thioesters	233
14-6. Compounds Containing the >C=S Group	235
14-7. Compounds Containing the S=O Groups	240
14-8. Compounds Containing $\text{-SO}_2\text{-}$ Groups	244
14-9. S-X Stretchings, X = O, N, F, Cl, Br	246
References	246

15. Organosilicon Compounds

15-1. The -SiH_3 Group	251
15-2. The $\text{-SiH}_2\text{-}$ Group	252
15-3. The Si-H Group	254
15-4. The Si-C Stretching	255
15-5. Si-C Groups	257
15-6. The Si-O Stretching	258
15-7. The Si-Si Stretching	259
15-8. Si-Halogen	259
References	260

16. Organophosphorus Compounds

16-1. PH Vibrations	263
16-2. The P=O Group	264
16-3. The P=S Group	266
16-4. The P-OH Group	268
16-5. Salts of Acids Containing Phosphorus	269
16-6. The P-O-P Group	270
16-7. The P-O-C Group	270
16-8. P-CH ₃ , P-CH ₂ , and P-Phenyl Groups	272
16-9. PN Groups	273
16-10. P-F, P-Cl and P-S Groups	274
References	275

17. Aromatic and Heteroaromatic Rings

17-1. Benzene Rings	277
17-2. The 1620–1400 cm^{-1} Ring Bands	279
17-3. The 1300–1000 cm^{-1} Region	282
17-4. The Aryl C–H Wag Vibrations	284
17-5. Ring Deformation Modes	290
17-6. Substituent-Sensitive Bands	291
17-7. Fused Ring Aromatics	294
17-8. Aromatic Heterocycles, Six-Membered Rings	295
17-9. Aromatic Heterocycles, Five-Membered Rings	301
References	304

18. Selected Infrared and Raman Spectra from the Sadtler Research Laboratories, Division of Bio-Rad Laboratories, Inc., for Compounds Discussed in Chapters 2–17

Instrumentation	307
Sample Preparation	308
Infrared Spectra	308
Index to Spectra	308
Spectra	312

Appendix One Infrared and Raman Spectra of Common Organic Compounds—From the Aldrich Library of FT-IR Spectra and the Dollish, Fateley and Bentley Collection

Index to Spectra	424
Spectra	425

Appendix Two Infrared and Raman Spectra of Selected Carbohydrate, Steroid, Organometallic, and Polymer Spectra from the Schrader Raman/Infrared Atlas of Organic Compounds

Index to Spectra	455
Spectra	457

Appendix Three A Summary of Characteristic Raman and Infrared Frequencies	
A. A Summary of Characteristic Raman Frequencies	477
B. Colthup Spectra-Structure Correlation Charts for IR Frequencies in the 4000-600 cm^{-1} Region	484
Alphabetical Name Index of Spectra	
Molecular Formula Index of Spectra	495
Index	499