

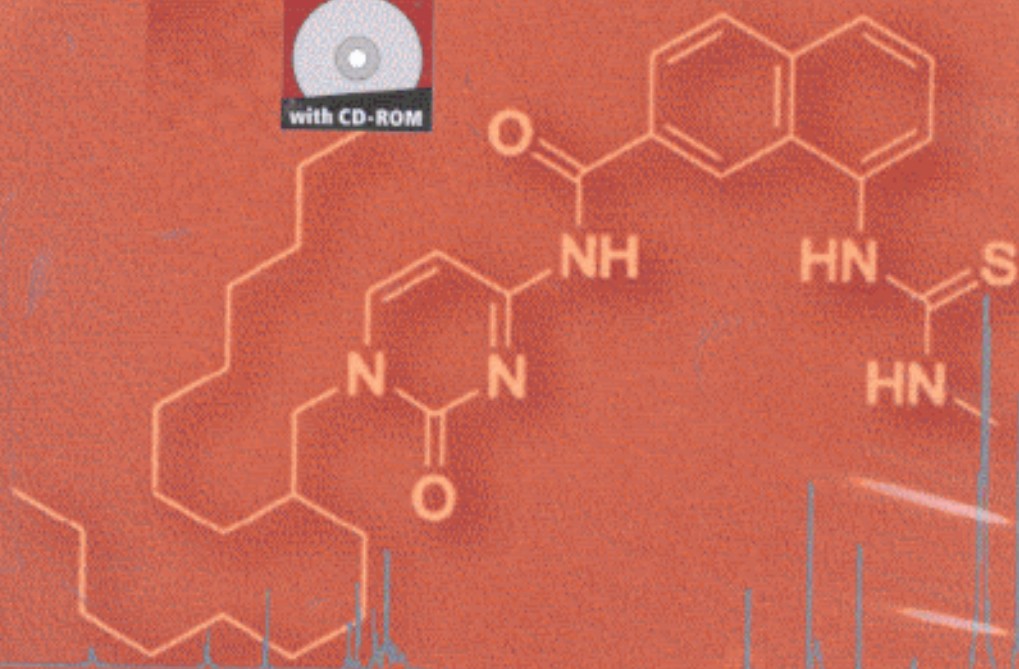
E. Pretsch P. Bühlmann
C. Affolter

Structure Determination of Organic Compounds

Tables of Spectral Data



with CD-ROM



Springer

Table of Contents

1 Introduction	1
1.1 Scope and Organization	1
1.2 Abbreviations and Symbols	3
2 Summary Tables	5
2.1 General Tables	5
2.1.1 Calculation of the Number of Double Bond Equivalents from the Molecular Formula	5
2.1.2 Properties of Selected Nuclei	6
2.2 ¹³ C NMR Spectroscopy	7
2.3 ¹ H NMR Spectroscopy	10
2.4 IR Spectroscopy	13
2.5 Mass Spectrometry	18
2.5.1 Average Masses of Naturally Occurring Elements with Exact Masses and Representative Relative Abundances of Isotopes	18
2.5.2 Ranges of Natural Isotope Abundances of Selected Elements	24
2.5.3 Isotope Patterns of Naturally Occurring Elements	25
2.5.4 Calculation of Isotope Distributions	26
2.5.5 Isotopic Abundances of Various Combinations of Chlorine, Bromine, Sulfur, and Silicon	28
2.5.6 Isotope Patterns of Combinations of Cl and Br	30
2.5.7 Indicators of the Presence of Heteratoms	31
2.5.8 Rules for Determining the Relative Molecular Weight (Mr)	33
2.5.9 Homologous Mass Series as Indications of Structural Type	34
2.5.10 Mass Correlation Table	36
2.5.11 References	46
2.6 UV/Vis Spectroscopy	47
3 Combination Tables	49
3.1 Alkanes, Cycloalkanes	49
3.2 Alkenes, Cycloalkenes	50
3.3 Alkynes	51
3.4 Aromatic Hydrocarbons	52
3.5 Heteroaromatic Compounds	53

3.6	Halogen Compounds	54
3.7	Oxygen Compounds	56
3.7.1	Alcohols and Phenols	56
3.7.2	Ethers	57
3.8	Nitrogen Compounds	59
3.8.1	Amines	59
3.8.2	Nitro Compounds	60
3.9	Thiols and Sulfides	62
3.10	Carbonyl Compounds	63
3.10.1	Aldehydes	63
3.10.2	Ketones	64
3.10.3	Carboxylic Acids	65
3.10.4	Carboxylic Esters and Lactones	66
3.10.5	Carboxylic Amides and Lactams	68
4	^{13}C NMR Spectroscopy	71
4.1	Alkanes	71
4.1.1	Chemical Shifts	71
4.1.2	Coupling Constants	80
4.1.3	References	81
4.2	Alkenes	82
4.2.1	Chemical Shifts	82
4.2.2	Coupling Constants	86
4.2.3	References	87
4.3	Alkynes	88
4.3.1	Chemical Shifts	88
4.3.2	Coupling Constants	89
4.3.3	References	89
4.4	Alicyclics	90
4.4.1	Chemical Shifts	90
4.4.2	Coupling Constants	95
4.4.3	References	95
4.5	Aromatic Hydrocarbons	96
4.5.1	Chemical Shifts	96
4.5.2	Coupling Constants	102
4.5.3	References	103
4.6	Heteroaromatic Compounds	104
4.6.1	Chemical Shifts	104
4.6.2	Coupling Constants	111
4.7	Halogen Compounds	112
4.7.1	Fluoro Compounds	112
4.7.2	Chloro Compounds	114
4.7.3	Bromo Compounds	115
4.7.4	Iodo Compounds	116
4.7.5	References	116
4.8	Alcohols, Ethers, and Related Compounds	117
4.8.1	Alcohols	117
4.8.2	Ethers	119

4.9	Nitrogen Compounds.....	121
4.9.1	Amines.....	121
4.9.2	Nitro and Nitroso Compounds.....	123
4.9.3	Nitrosamines.....	124
4.9.4	Imines and Oximes.....	124
4.9.5	Hydrazones and Carbodiimides.....	125
4.9.6	Nitriles and Isonitriles.....	126
4.9.7	Isocyanates, Thiocyanates and Isothiocyanates.....	127
4.9.8	References.....	127
4.10	Sulfur-Containing Functional Groups.....	128
4.10.1	Thiols.....	128
4.10.2	Sulfides.....	128
4.10.3	Disulfides and Sulfonium Salts.....	130
4.10.4	Sulfoxides and Sulfones.....	130
4.10.5	Sulfonic and Sulfinic Acids and Derivatives.....	131
4.10.6	Sulfurous and Sulfuric Acid Derivatives.....	131
4.10.7	Sulfur-Containing Carbonyl Derivatives.....	132
4.11	Carbonyl Compounds.....	133
4.11.1	Aldehydes.....	133
4.11.2	Ketones.....	134
4.11.3	Carboxylic Acids and Carboxylates.....	136
4.11.4	Esters and Lactones.....	138
4.11.5	Amides and Lactams.....	140
4.11.6	Miscellaneous Carbonyl Derivatives.....	142
4.12	Miscellaneous Compounds.....	144
4.12.1	Derivatives of Group IV Elements.....	144
4.12.2	Phosphorus Compounds.....	145
4.12.3	Miscellaneous Organometallic Compounds.....	147
4.13	Natural Products.....	148
4.13.1	Amino Acids.....	148
4.13.2	Carbohydrates.....	152
4.13.3	Nucleotides and Nucleosides.....	154
4.13.4	Steroids.....	156
4.14	Spectra of Solvents and Reference Compounds.....	157
4.14.1	^{13}C NMR Spectra of Common Deuterated Solvents.....	157
4.14.2	^{13}C NMR Spectra of Secondary Reference Compounds.....	159
4.14.3	^{13}C NMR Spectrum of a Mixture of Common Nondeuterated Solvents.....	160
5	^1H NMR Spectroscopy.....	161
5.1	Alkanes.....	161
5.1.1	Chemical Shifts.....	161
5.1.2	Coupling Constants.....	166
5.1.3	References.....	167
5.2	Alkenes.....	168
5.2.1	Substituted Ethylenes.....	168
5.2.2	Dienes.....	174
5.3	Alkynes.....	175

5.3.1	Chemical Shifts and Coupling Constants.....	175
5.4	Alicyclics.....	176
5.5	Aromatic Hydrocarbons.....	180
5.6	Heteroaromatic Compounds.....	186
5.6.1	Non-Condensed Heteroaromatic Rings.....	186
5.6.2	Condensed Heteroaromatic Rings.....	193
5.7	Halogen Compounds.....	198
5.7.1	Fluoro Compounds.....	198
5.7.2	Chloro Compounds.....	199
5.7.3	Bromo Compounds.....	200
5.7.4	Iodo Compounds.....	201
5.8	Alcohols, Ethers, and Related Compounds.....	202
5.8.1	Alcohols.....	202
5.8.2	Ethers.....	204
5.9	Nitrogen Compounds.....	207
5.9.1	Amines.....	207
5.9.2	Nitro and Nitroso Compounds.....	210
5.9.3	Nitrosamines, Azo, and Azoxy Compounds.....	210
5.9.4	Imines, Oximes, Hydrazones, and Azines.....	211
5.9.5	Nitriles and Isonitriles.....	212
5.9.6	Cyanates, Isocyanates, Thiocyanates, and Isothiocyanates.....	213
5.10	Sulfur-Containing Functional Groups.....	214
5.10.1	Thiols.....	214
5.10.2	Sulfides.....	215
5.10.3	Disulfides and Sulfonium Salts.....	216
5.10.4	Sulfoxides and Sulfones.....	216
5.10.5	Sulfonic, Sulfinic, Sulfurous, and Sulfuric Acids and Derivatives.....	217
5.10.6	Thiocarboxylate Derivatives.....	217
5.11	Carbonyl Compounds.....	218
5.11.1	Aldehydes.....	218
5.11.2	Ketones.....	219
5.11.3	Carboxylic Acids and Carboxylates.....	220
5.11.4	Esters and Lactones.....	221
5.11.5	Amides and Lactams.....	223
5.11.6	Miscellaneous Carbonyl Derivatives.....	226
5.12	Miscellaneous Compounds.....	228
5.12.1	Silicon Compounds.....	228
5.12.2	Phosphorus Compounds.....	229
5.12.3	Miscellaneous Compounds.....	232
5.13	Natural Products.....	233
5.13.1	Amino Acids.....	233
5.13.2	Carbohydrates.....	236
5.13.3	Nucleotides and Nucleosides.....	237
5.13.4	References.....	239
5.14	Spectra of Solvents and Reference Compounds.....	240
5.14.1	¹ H NMR Spectra of Common Deuterated Solvents.....	240
5.14.2	¹ H NMR Spectra of Secondary Reference Compounds.....	242

5.14.3	^1H NMR Spectrum of a Mixture of Common Nondeuterated Solvents.....	243
6	IR Spectroscopy.....	245
6.1	Alkanes.....	245
6.2	Alkenes.....	248
6.2.1	Monoenes.....	248
6.2.2	Allenes.....	251
6.3	Alkynes.....	252
6.4	Alicyclics.....	253
6.5	Aromatic Hydrocarbons.....	255
6.6	Heteroaromatic Compounds.....	258
6.7	Halogen Compounds.....	260
6.7.1	Fluoro Compounds.....	260
6.7.2	Chloro Compounds.....	261
6.7.3	Bromo Compounds.....	262
6.7.4	Iodo Compounds.....	262
6.8	Alcohols, Ethers, and Related Compounds.....	263
6.8.1	Alcohols and Phenols.....	263
6.8.2	Ethers, Acetals, Ketals.....	264
6.8.3	Epoxides.....	266
6.8.4	Peroxides and Hydroperoxides.....	267
6.9	Nitrogen Compounds.....	268
6.9.1	Amines and Related Compounds.....	268
6.9.2	Nitro and Nitroso Compounds.....	270
6.9.3	Imines and Oximes.....	272
6.9.4	Azo Compounds.....	274
6.9.5	Nitriles and Isonitriles.....	275
6.9.6	Diazo Compounds.....	276
6.9.7	Cyanates and Isocyanates.....	277
6.9.8	Thiocyanates and Isothiocyanates.....	278
6.10	Sulfur-Containing Functional Groups.....	280
6.10.1	Thiols and Sulfides.....	280
6.10.2	Sulfoxides and Sulfones.....	281
6.10.3	Thiocarbonyl Derivatives.....	283
6.10.4	Thiocarbonic Acid Derivatives.....	283
6.11	Carbonyl Compounds.....	286
6.11.1	Aldehydes.....	286
6.11.2	Ketones.....	287
6.11.3	Carboxylic Acids.....	290
6.11.4	Esters and Lactones.....	292
6.11.5	Amides and Lactams.....	295
6.11.6	Acid Anhydrides.....	298
6.11.7	Acid Halides.....	300
6.11.8	Carbonic Acid Derivatives.....	301
6.12	Miscellaneous Compounds.....	304
6.12.1	Silicon Compounds.....	304
6.12.2	Phosphorus Compounds.....	305

6.12.3	Boron Compounds.....	308
6.13	Amino Acids.....	309
6.14	Solvents, Suspension Media, and Interferences.....	310
6.14.1	Infrared Spectra of Common Solvents.....	310
6.14.2	Infrared Spectra of Suspension Media.....	311
6.14.3	Interferences in Infrared Spectra.....	312
7	Mass Spectrometry.....	313
7.1	Alkanes.....	313
7.1.1	Unbranched Alkanes.....	313
7.1.2	Branched Alkanes.....	313
7.1.3	References.....	314
7.2	Alkenes.....	315
7.2.1	Unbranched Alkenes.....	15
7.2.2	Branched Alkenes.....	315
7.2.3	Polyenes and Polyynes.....	316
7.2.4	References.....	316
7.3	Alkynes.....	317
7.3.1	Aliphatic Alkynes.....	317
7.3.2	References.....	317
7.4	Alicyclic Hydrocarbons.....	318
7.4.1	Cyclopropanes.....	318
7.4.2	Saturated Monocyclic Alicyclics.....	319
7.4.3	Polycyclic Alicyclics.....	319
7.4.4	Cyclohexenes.....	319
7.4.5	References.....	320
7.5	Aromatic Hydrocarbons.....	321
7.5.1	Aromatic Hydrocarbons.....	321
7.5.2	Alkylsubstituted Aromatic Hydrocarbons.....	321
7.5.3	References.....	322
7.6	Heteroaromatic Compounds.....	323
7.6.1	General Characteristics.....	323
7.6.2	Furans.....	323
7.6.3	Thiophenes.....	323
7.6.4	Pyrroles.....	324
7.6.5	Pyridines.....	324
7.6.6	N-Oxides of Pyridines and Quinolines.....	325
7.6.7	Pyridazines and Pyrimidines.....	325
7.6.8	Pyrazines.....	326
7.6.9	Indoles.....	326
7.6.10	Quinolines.....	326
7.6.11	Cinnoline.....	327
7.6.12	References.....	327
7.7	Halogen.....	328
7.7.1	Saturated Aliphatic Halides.....	328
7.7.2	Polyhaloalkanes.....	329
7.7.3	Aromatic Halides.....	329
7.7.4	References.....	329

7.8	Alcohols.....	330
7.8.1	Aliphatic Alcohols.....	330
7.8.2	Alicyclic Alcohols.....	331
7.8.3	Unsaturated Aliphatic Alcohols.....	331
7.8.4	Vicinal Glycols.....	331
7.8.5	Aliphatic Hydroperoxides.....	332
7.8.6	Phenols.....	332
7.8.7	Benzyl.....	332
7.8.8	Aliphatic Ethers.....	333
7.8.9	Unsaturated Ethers.....	334
7.8.10	Alkyl Cycloalkyl Ethers.....	335
7.8.11	Cyclic Ethers.....	335
7.8.12	Aliphatic Epoxides.....	336
7.8.13	Methoxybenzenes.....	337
7.8.14	Alkyl Aryl Ethers.....	337
7.8.15	Aromatic Ethers.....	337
7.8.16	Aliphatic Peroxides.....	337
7.8.17	References.....	338
7.9	Nitrogen Compounds.....	339
7.9.1	Saturated Aliphatic Amines.....	339
7.9.2	Cycloalkylamines.....	339
7.9.3	Cyclic Amines.....	340
7.9.4	Piperazines.....	341
7.9.5	Aromatic Amines.....	341
7.9.6	Aliphatic Nitro Compounds.....	341
7.9.7	Aromatic Nitro Compounds.....	342
7.9.8	Diazo.....	342
7.9.9	Azobenzenes.....	342
7.9.10	Aliphatic Azides.....	342
7.9.11	Aromatic Azides.....	343
7.9.12	Aliphatic Nitriles.....	343
7.9.13	Aromatic Nitriles.....	344
7.9.14	Aliphatic Isonitriles (R-NC).....	344
7.9.15	Aromatic Isonitriles (R-NC).....	344
7.9.16	Aliphatic Cyanates (R-OCN).....	345
7.9.17	Aromatic Cyanates (R-OCN).....	345
7.9.18	Aliphatic Isocyanates (R-NCO).....	345
7.9.19	Aromatic Isocyanates (R-NCO).....	346
7.9.20	Aliphatic Thiocyanates (R-SCN).....	346
7.9.21	Aromatic Thiocyanates (R-SCN).....	347
7.9.22	Aliphatic Isothiocyanates (R-NCS).....	347
7.9.23	Aromatic Isothiocyanates (R-NCS).....	347
7.9.24	References.....	348
7.10	Sulfur-Containing Functional Groups.....	349
7.10.1	Aliphatic Thiols.....	349
7.10.2	Aromatic Thiols.....	349
7.10.3	Aliphatic Sulfides.....	350
7.10.4	Alkyl Vinyl Sulfides.....	350
7.10.5	Cyclic Sulfides.....	351

7.10.6	Aromatic Sulfides.....	351
7.10.7	Disulfides.....	351
7.10.8	Aliphatic Sulfoxides.....	352
7.10.9	Alkyl Aryl and Diaryl Sulfoxides.....	352
7.10.10	Aliphatic Sulfones.....	353
7.10.11	Cyclic Sulfones.....	354
7.10.12	Alkyl Aryl Sulfones.....	354
7.10.13	Diaryl Sulfones.....	355
7.10.14	Aromatic Sulfonic Acids.....	355
7.10.15	Alkylsulfonic Acid Esters.....	355
7.10.16	Arylsulfonic Acid Esters.....	356
7.10.17	Aromatic Sulfonamides.....	356
7.10.18	Thiocarboxylic Acid S-Esters.....	357
7.10.19	References.....	357
7.11	Carbonyl Compounds.....	358
7.11.1	Aliphatic Aldehydes.....	358
7.11.2	Unsaturated Aliphatic Aldehydes.....	358
7.11.3	Aromatic Aldehydes.....	358
7.11.4	Aliphatic Ketones.....	359
7.11.5	Unsaturated Ketones.....	359
7.11.6	Alicyclic Ketones.....	359
7.11.7	Aromatic Ketones.....	360
7.11.8	Aliphatic Carboxylic Acids.....	360
7.11.9	Aromatic Carboxylic Acids.....	361
7.11.10	Carboxylic Acid Anhydrides.....	361
7.11.11	Saturated Aliphatic Esters.....	361
7.11.12	Unsaturated Esters.....	362
7.11.13	Esters of Aromatic Acids.....	363
7.11.14	Lactones.....	364
7.11.15	Aliphatic Amides.....	364
7.11.16	Amides of Aromatic Carboxylic Acids.....	365
7.11.17	Anilides.....	365
7.11.18	Lactams.....	365
7.11.19	Imides.....	367
7.11.20	References.....	368
7.12	Miscellaneous Compounds.....	369
7.12.1	Trialkylsilyl Ethers.....	369
7.12.2	Alkyl Phosphates.....	369
7.12.3	Aliphatic Phosphines.....	369
7.12.4	Aromatic Phosphines and Phosphine Oxides.....	370
7.12.5	References.....	370
7.13	Mass Spectra of Common Solvents and Matrix Compounds.....	371
7.13.1	Electron Impact Ionization Mass Spectra of Common Solvents.....	371
7.13.2	Spectra of Common FAB MS Matrix and Calibration Compounds.....	374
7.13.3	Spectra of Common MALDI MS Matrix Compounds.....	380
7.13.4	References.....	383

8 UV/Vis Spectroscopy	385
8.1 Correlation Between Wavelength of Absorbed Radiation and Observed Color.....	385
8.2 UV/Vis Absorption of Simple Chromophores.....	385
8.3 UV/Vis Absorption of Conjugated Alkenes.....	387
8.3.1 UV Absorption of Dienes and Polyenes	387
8.3.2 UV Absorption of α,β -Unsaturated Carbonyl Compounds	388
8.4 UV/Vis Absorption of Aromatic Compounds.....	390
8.4.1 UV Absorption of Monosubstituted Benzenes	390
8.4.2 UV Absorption of Substituted Benzenes.....	391
8.4.3 UV Absorption of Aromatic Carbonyl Compounds.....	392
8.5 UV/Vis Reference Spectra.....	393
8.5.1 UV/Vis Spectra of Alkenes and Alkynes	393
8.5.2 UV/Vis Spectra of Aromatic Compounds.....	394
8.5.3 UV/Vis Spectra of Heteroaromatic Compounds	399
8.5.4 UV/Vis Spectra of Miscellaneous Compounds	401
8.5.5 UV/Vis Spectra of Nucleotides.....	403
8.6 UV/Vis Absorption of Common Solvents.....	404
Subject Index	406