

TABLE OF CONTENTS

SECTION A _ SPECTROSCOPIC AIDS

Part I _ Infrared Spectroscopy

Terms. Symbols and Definitions	A-5
Conversion Table. Wavelength – Wavenumber (μ to cm^{-1})	A-6
Conversion Table. Percent Transmittance – Absorbance	A-8
IR Transmission Characteristics of Crystals	A-12
Useful Solvents in the Infrared	A-13
Calibration of Infrared Spectrometers and Cells	A-17
Specifications for Infrared Reference Spectra (Coblentz Society)	A-20
Group Frequency Correlation Charts	A-23
Tracking Down Spurious Bands in Infrared Analysis	A-49
Bibliography of Useful References	A-52

Part II _ Ultraviolet Spectroscopy

Terms. Symbols and Definitions	A-55
Conversion Table. Wavelength – Wavenumber (nm to cm^{-1})	A-56
UV Transmission Characteristics of Optical Materials	A-57
Ultraviolet Cut-off Point for Common Solvents	A-58
Calibration of UV Spectrometers	A-59
Ultraviolet Absorption of Characteristic Chromophores	A-63
Rules for Estimating Ultraviolet Absorption for Various Groups	A-64
Bibliography of Useful References	A-65

Part III _ Nuclear Magnetic Resonance Spectroscopy

Terms. Symbols and Definitions	A-69
NMR Active Nucleii	A-70
Nuclear Spins. Moments and Magnetic Resonance Frequencies	A-71
Common NMR Solvents	A-75
Resolution and sensitivity of NMR Spectrometers	A-79
Chemical Shift Charts. Rules for Estimating Substituent Effects and Coupling Constants	A-81
Bibliography of Useful References	A-92

Part IV _ Mass Spectrometry

Terms. Symbols and Definitions	A-95
Calibration of Mass Spectrometers	A-96
Interpretation Procedure. Natural Abundances of Common Isotopes and Elemental Composition	A-98
Common Ion Fragments or Neutral Species	A-99
Bibliography of Useful References	A-105

TABLE OF CONTENTS Continued

SECTION B _ MASTER DATA TABLE

Spectral Data and Physical Constants for Organic Compounds

Explanation of Table	B-1
Rules for Naming Compounds	B-2
Compound Name/Synonym Directory	B-11
Symbols and Abbreviations	B-90
Spectral Data and Physical Constants for Organic Compounds, Table I	B-91
References to Original Literature Source – UV Data, Table 2	B-997
Coden Literature List	B-1001
Structural Formulas of Organic Compounds	B-1005

SECTION C _ INDEXES

Part I _ Physical Constants

Empirical Formula Index of Organic Compounds	C-1
Empirical Formula Index of Organic Compounds: Hydrates	C-15
Empirical Formula Index of Organic Compounds: Halide Salts	C-16
Empirical Formula Index of Organic Compounds: Other Salts	C-17
Molecular Weight Index of Organic Compounds	C-18
Melting Point Index of Organic Compounds	C-32
Boiling Point Index of Organic Compounds	C-39

Part II _ Chemical Structure and Sub-structure Index (Wiswesser Line Notation)

Explanation of Index	C-45
Reference List of Wiswesser Line Formula Notation Symbols	C-47
Dictionary of Frequently Found Sub-Structures	C-48
WLN Permuted Index	C-51

Part III _ Infrared

Numerical Index of Source Curves	C-252
Spectral Data Index	C-270

Part IV _ Ultraviolet

Numerical Index of Source Curves	C-417
Spectral Data Index	C-424

TABLE OF CONTENTS Continued

Part V — Nuclear Magnetic Resonance

Numerical Index of Source Curves	C-455
Spectral Data Index: Low Field to High Field	C-464
Spectral Data Index: High Field to Low Field	C-490

Part VI — Mass Spectrometry

Numerical Index of Source Curves	C-515
Spectral Data Index	C-522
Molecular Weight Index to Chlorine Containing Compounds	C-550
Molecular Weight Index to Bromine Containing Compounds	C-552
Molecular Weight Index to Nitrogen Containing Compounds	C-553
Molecular Weight Index to Sulfur Containing Compounds	C-557