

# Contents

<b>Foreword, Norman Wright</b>	<b>vii</b>
<b>Preface</b>	<b>ix</b>
<b>1. Infrared Radiation: Description and Simple Theory of Absorption by Molecules, David N. Kendall</b>	<b>1</b>
Introduction	1
The Empirical Approach	2
The Nature of Infrared Radiation	2
Simple Theory of Infrared Absorption by Molecules	10
<b>2. Survey of Practical Information, David N. Kendall</b>	<b>31</b>
Infrared Spectra of Molecules in Different Phases	31
Types of Molecular Vibrations	39
Group Frequencies	41
Qualitative Analysis	52
Quantitative Analysis	56
Shifts in Group Frequencies	69
The Limitations of Infrared Spectroscopy	82
<b>3. Instrumentation, L. W. Herscher</b>	<b>88</b>
Historical	88
Infrared Spectrometer Components	89
Practical Spectrometers	111
Electronic Systems and Operating Adjustments	123
Accessories for Special Samples	128
Instrumentation for the Far Infrared	131

<b>4. Sample Preparation Procedures, David N. Kendall</b>	<b>136</b>
Importance of Sample Preparation	136
Solids	136
Preparation, Use, and Care of Absorption Cells	151
Liquids and Solutions	156
Vapors	158
Films	160
Special Sampling Techniques	160
<b>5. A General Procedure for Qualitative Interpretation of Infrared Spectra, David N. Kendall</b>	<b>166</b>
Value of Sample History	166
Spectral Interpretation Procedure	167
Helpful Rules of Thumb	172
Interpretation of Spectra — Examples	173
Outline of a General Procedure for Qualitative Interpretation of Infrared Spectra	182
<b>6. Infrared on the Chemist's Bench, R. D. Moss, W. J. Potts, Jr.</b>	<b>185</b>
Introduction	185
Instrumentation and Experimental Techniques	187
Qualitative Analysis	196
Interpretation of Infrared Spectra: The Group Frequencies	203
Quantitative Analysis	214
<b>7. Pharmaceutical Applications of Infrared Spectroscopy, James L. Johnson, Robert W. Rinehart and C. Leroy Graham</b>	<b>222</b>
Introduction	222
Techniques	223
The Spectroscopists' Reference Library	226
Quality Control	230
Patents	238
<b>8. Application of Infrared Spectroscopy to Polymers, J. L. Koenig</b>	<b>245</b>
Introduction	245
Theory of Polymer Spectra	246
Sampling Techniques	251
Characterizing Macromolecular Structure	253

Applications of IR spectroscopy to Polymer Structure Elucidation	255
Infrared Characterization of the Chemical Reactions of Polymers	260
Quantitative IR Measurements on Polymer Systems	261
Configuration of the Chemical Repeat Unit in the Polymer Chain	268
Conformation of the Polymer Chain	273
Conclusions	280
9. Infrared Analysis of Essential Oils, Related Products, and Cos- metics, <i>James A. Rogers, Jr., and Zoltan E. Toth</i>	285
Introduction	285
Nature of the Industry	288
Utilization of Infrared in the Industry	289
Applications of Infrared	293
A General Procedure for Qualitative Infrared Investigations	308
Types of Infrared Laboratory Organization	309
The Future of Infrared	311
10. Infrared in Coal Structure Research, <i>R. A. Friedel</i>	312
Introduction	312
Experimental Techniques	314
Structure Assignments	319
Other Infrared Methods	326
Coal Extracts and Distillates	327
Reaction Products	328
Chars of Model Compounds	332
High Energy Effects	335
Other Studies	337
Aromaticity	338
Conclusions	339
11. Infrared in the Regulatory Agencies, <i>Jonas Carol and Alma L. Hayden</i>	344
Introduction	344
Identification of Unknown Pharmaceuticals	346
Use of Infrared by the Federal Bureau of Investigation	367
Development and Application of New Techniques	367

<b>12. Infrared in the Industrial Laboratory, Robert O. Crisler</b>	<b>377</b>
Introduction	377
Applications	378
Techniques	383
Qualitative Analysis and the Reference Spectra File	387
Setting Up an Industrial Infrared Laboratory	390
Summary	396
<b>13. Infrared Plant Stream Analyzers, A. M. Bartz and H. D. Ruhl</b>	<b>398</b>
Introduction	398
Nondispersive Analyzers	400
Dispersive Analyzers	415
Bandpass Interference Filter Analyzers	429
Optimization of Sample Cell Path Length	430
Future Trends	433
<b>14. Microtechniques Using Miniaturized Diamond Optics, Ellis R. Lippincott, Linda S. Whatley and H. C. Duecker</b>	<b>435</b>
Introduction	435
The Miniature Diamond Cell	436
Application of the Diamond Cell as a Routine Method of Obtaining Infrared Spectra of Solids and Liquids	443
Application of the Diamond Cell in High-Pressure Studies	447
The Microscope Spectrophotometer and its Applications	453
Some Additional Applications of the Diamond Cell	458
<b>15. Attenuated Total Reflectance, Stanley E. Polchlopek</b>	<b>462</b>
Introduction	462
The Essence of ATR	463
ATR Instrumentation	465
Sample Techniques	466
Applications	468
The Future of ATR	478
<b>16. Microsampling Techniques, David N. Kendall</b>	<b>485</b>
Introduction	485
Microsampling for Solids	485
Microsampling for Liquids and Solutions	494
Microsampling for Gases	495

<b>17. Inorganic Applications of Infrared Spectroscopy, David N. Kendall</b>	<b>497</b>
Introduction	497
Applications of Infrared to Inorganics	499
<b>18. The Use of Computers in Spectroscopy, Abraham Savitzky</b>	<b>509</b>
Prologue	509
Section I. NUMERICAL PROCESSING OF SPECTRAL DATA	509
Introduction	509
Programming	511
Applications	515
Section 2. SPECTRAL LIBRARIES AND THE IDENTIFICATION OF A SPECTRUM	529
The Identification of a Spectrum	529
Spectral Indexes by Machine Methods	530
Spectral Indexes by Nonmachine Methods	531
Computer Techniques for Searching the IBM Card File	531
Conclusion	532
<b>Index</b>	<b>536</b>