

Contents

Study Guide	xiii
Supporting Practical Work	xv
Bibliography	xvii
Acknowledgements	xix
1. Introduction	1
1.1 General Introduction	1
1.2 Electromagnetic Radiation	2
1.3 Distribution and Lifetimes of Energy States	6
1.3.1 Population of Energy States	6
1.3.2 Lifetimes of Excited States	8
1.4 Molecular Vibrations	9
1.4.1 Normal Modes of Vibration	9
1.4.2 Intensity of Infrared Bands	15
2. Instrumentation	19
2.1 Introduction	19
2.2 Representation of Spectra	19
2.3 Dispersive Spectrometers	22
2.3.1 Monochromators	22
2.3.2 Double-beam Instruments	23
2.3.3 Sources and Detectors	24
2.3.4 Limitations	24
2.4 Fourier-transform Infrared Spectrometers	25
2.4.1 The Michelson Interferometer	26
2.4.2 Fourier Transformation	28
2.4.3 Sources and Detectors	29
2.4.4 The Moving Mirror	29
2.4.5 Signal Averaging	31

2.4.6 Advantages of Fourier-transform Infrared Spectroscopy	32
2.4.7 Computers	33
3. Sampling Methods	35
3.1 Introduction	35
3.2 Transmission Methods	35
3.2.1 Liquids and Solutions	35
3.2.2 Solids	42
3.3 Reflectance Methods	46
3.3.1 Attenuated Total Reflectance Spectroscopy	46
3.3.2 Specular Reflectance	50
3.3.3 Diffuse Reflectance	51
3.4 Microsampling Methods	52
3.5 Gas Chromatography-Infrared Spectroscopy	54
3.6 Temperature Studies	55
3.7 Photoacoustic Spectroscopy	55
4. Spectrum Interpretation	59
4.1 Introduction	59
4.2 Group Frequencies	59
4.2.1 The X—H Stretching Region ($4000\text{--}2500\text{ cm}^{-1}$)	59
4.2.2 The Triple Bond Region ($2500\text{--}2000\text{ cm}^{-1}$)	60
4.2.3 The Double Bond Region ($2000\text{--}1500\text{ cm}^{-1}$)	61
4.2.4 The Fingerprint Region ($1500\text{--}600\text{ cm}^{-1}$)	61
4.3 Summary of Characteristic Frequencies	62
4.3.1 Alkanes	62
4.3.2 Alkenes	63
4.3.3 Alkynes	64
4.3.4 Aromatic Compounds	64
4.3.5 Alcohols, Phenols and Ethers	65
4.3.6 Amines	66
4.3.7 Other Nitrogen Compounds	66
4.3.8 Aldehydes and Ketones	67
4.3.9 Other Carbonyl Compounds	67
4.3.10 Sulfur Compounds	68
4.3.11 Halogen Compounds	69
4.3.12 Phosphorus Compounds	69
4.4 Complicating Factors	71
4.4.1 Overtone and Combination Bands	71

4.4.2 Fermi Resonance	75
4.4.3 Hydrogen Bonding	75
4.4.4 Coupling	78
4.5 Identification of Unknown Compounds	79
 5. Quantitative Analysis	 85
5.1 Introduction	85
5.2 Spectrum Manipulation	85
5.2.1 Baseline Correction	86
5.2.2 Smoothing	86
5.2.3 Difference Spectra	87
5.2.4 Derivatives	88
5.2.5 Deconvolution	90
5.2.6 Curve-fitting	92
5.3 Pathlength Calibration	93
5.4 Determination of Concentration	95
5.5 Simple Analysis	98
5.5.1 Analysis of Liquids and Solutions	98
5.5.2 Analysis of Solid Samples	102
5.6 Multicomponent Analysis	103
5.6.1 Analysis of a Three-component Drug Mixture	103
5.6.2 Analysis of Fermentation Broths	105
5.6.3 Determination of the <i>Trans</i> -unsaturation Content of Fats	107
5.6.4 Multivariate Calibration Methods	109
 6. Applications	 113
6.1 Introduction	113
6.2 Proteins and Peptides	113
6.2.1 Interpretation of the Spectra of Proteins and Peptides	113
6.2.2 Analysis of the Amide I Band	116
6.2.3 Protein Adsorption Studies	127
6.3 Lipids	127
6.3.1 Interpretation of the Spectra of Lipids	127
6.3.2 Temperature Studies	131
6.3.3 Analysis of the Lipid Carbonyl Band	132
6.3.4 Analysis of Blood Serum	133
6.4 Biomembranes	134
6.4.1 Interpretation of the Spectra of Biomembranes	134
6.4.2 Analysis of Membrane Proteins	134

6.4.3 Analysis of Membrane Lipids	137
6.5 Animal Tissue	139
6.5.1 Analysis of Malignant Tissues	139
6.5.2 Analysis of Skin	142
6.6 Carbohydrates	143
6.6.1 Sugars	143
6.6.2 Nucleic Acids	144
6.7 Pharmaceuticals	146
6.7.1 Interpretation of the Spectra of Drugs	146
6.7.2 Penicillins	147
6.7.3 GC-IR Analysis of Amphetamines	148
6.8 Foods	149
6.8.1 Interpretation of the Spectra of Foods	149
6.8.2 Analysis of Wine	149
6.8.3 Analysis of Artificial Sweeteners	150
6.9 Plant Material	151
Self-assessment Questions and Responses	155
Units of Measurement	181
Index	187