
Modern Raman Spectroscopy – A Practical Approach

Ewen Smith

Strathclyde University, Glasgow

Geoffrey Dent

Intertek ASG and UMIST, Manchester



John Wiley & Sons, Ltd

Contents

Preface	ix
Acknowledgements	xi
CHAPTER 1 INTRODUCTION, BASIC THEORY AND PRINCIPLES	1
1.1 Introduction	1
1.2 Basic Theory	2
1.3 Molecular Vibrations	8
1.4 Summary	20
CHAPTER 2 THE RAMAN EXPERIMENT – RAMAN INSTRUMENTATION, SAMPLE PRESENTATION, DATA HANDLING AND PRACTICAL ASPECTS OF INTERPRETATION	23
2.1 Introduction	23
2.2 Choice of Instrument	24
2.3 Visible Excitation	24
2.4 NIR Excitation	30
2.5 Raman Sample Preparation and Handling	31
2.6 Sample Mounting Accessories	41
2.7 Microscopy	45
2.8 Calibration	51
2.9 Data Handling, Manipulation and Quantitation	53
2.10 Approach to Qualitative Interpretation	61
2.11 Summary	67
CHAPTER 3 THE THEORY OF RAMAN SPECTROSCOPY	71
3.1 Introduction	71
3.2 Absorption and Scattering	72
3.3 States of a System and Hooke's Law	74
3.4 The Nature of Polarizability and the Measurement of Polarization	76

3.5	The Basic Selection Rule	80
3.6	Number and Symmetry of Vibrations	80
3.7	Symmetry Elements and Point Groups	82
3.8	The Mutual Exclusion Rule	86
3.9	The Kramer Heisenberg Dirac Expression	86
3.10	Lattice Modes	90
3.11	Conclusions	91
CHAPTER 4 RESONANCE RAMAN SCATTERING		93
4.1	Introduction	93
4.2	Theoretical Aspects	94
4.3	Practical Aspects	101
4.4	Examples of the Use of Resonance Raman Scattering	103
4.5	Conclusions	112
CHAPTER 5 SURFACE-ENHANCED RAMAN SCATTERING AND SURFACE-ENHANCED RESONANCE RAMAN SCATTERING		113
5.1	Introduction	113
5.2	Theory	116
5.3	Electromagnetic and Charge Transfer Enhancement	117
5.4	Selection Rules	121
5.5	Applications of SERS	122
5.6	Applications of SERRS	126
5.7	The Basic Method	127
CHAPTER 6 APPLICATIONS		135
6.1	Introduction	135
6.2	Inorganics and Minerals	135
6.3	Art and Archaeology	143
6.4	Polymers and Emulsions	143
6.5	Colour	149
6.6	Electronics Applications	158
6.7	Biological and Pharmaceutical Applications	160
6.8	Forensic Applications	166
6.9	Plant Control and Reaction Following	167
6.10	Summary	172
CHAPTER 7 MORE ADVANCED RAMAN SCATTERING TECHNIQUES		181
7.1	Flexible Optics	182
7.2	Tuneable Lasers, Frequency Doubling and Pulsed Lasers	187
7.3	Spatially Resolved Systems	189

<i>Contents</i>	vii
7.4 Nonlinear Raman Spectroscopy	191
7.5 Time Resolved Scattering	196
7.6 Raman Optical Activity	198
7.7 UV Excitation	199
7.8 Conclusions	201
Index	203