

Contents

PREFACE	v
LIST OF CONTRIBUTORS	ix

PART I. THE DETERMINATION OF MOLECULAR SIZE

1. Phase Properties of Small Molecules BY H. F. HERBRANDSON AND F. C. NACHOD		3
NACHOD		3
1.1. Introduction		3
1.2. Melting Points		3
1.3. Boiling Points		16
1.4. Molar Volume		19
1.5. Parachor		20
References		21
2. Equilibrium and Dynamic Properties of Large Molecules BY P. JOHNSON		25
2.1. Introduction		25
2.2. Osmotic Pressure		28
2.3. Sedimentation Equilibrium		41
2.4. Sedimentation Velocity		44
2.5. Diffusion		55
2.6. Viscosity		59
2.7. Comparison of Results Obtained by Different Methods		64
References		67

PART II. THE DETERMINATION OF MOLECULAR PATTERN

3. Optical Rotation BY W. KLYNE		73
3.1. Introduction		73
3.2. Conventions		74
3.3. Experimental Methods		76
3.4. Principles of Optical Rotation		78
3.5. Simple Acyclic Compounds		83
3.6. Carbohydrates		94
3.7. Steroids		108
3.8. Triterpenoids		118
3.9. Diterpenoids		122
3.10. Other Groups of Compounds		125
References		126
4. Ultraviolet and Visible Light Absorption BY E. A. BRAUDE		131
4.1. Introduction		131
4.2. Fundamental Concepts and Symbols		133
4.3. Experimental Methods and Evaluation of Data		139
4.4. Survey of Data		144
4.5. General Applications to Structural Analysis		158
4.6. Special Applications		176
References		186

5. Infrared Light Absorption BY R. C. GORE	195
5.1. Introduction	195
5.2. Experimental Methods	196
5.3. General Applications	202
5.4. Applications to the Study of Macromolecules (BY E. S. WAIGHT)	219
References	228
6. Raman Spectra BY FORREST F. CLEVELAND	231
6.1. Introduction	231
6.2. Experimental Methods	232
6.3. Survey of Data	235
6.4. Applications to the Determination of Structure	239
6.5. Determination of Thermodynamic Properties	255
6.6. Conclusion	256
References	257
7. Magnetic Susceptibilities BY CLYDE A. HUTCHISON, JR.	259
7.1. The Theory of Magnetic Susceptibility	259
7.2. Applications to the Study of Organic Compounds. Static Fields	282
7.3. Applications to the Study of Organic Compounds. Alternating Fields	308
References	319
PART III. THE DETERMINATION OF MOLECULAR FINE-STRUCTURE	
8. Surface Films BY E. STENHAGEN	325
8.1. Introduction	325
8.2. The Technique of Surface Film Measurements	326
8.3. The Relation Between the Structure of Organic Molecules and the Mechanical Properties of Their Surface Films	328
8.4. The Relation Between the Structure of Organic Molecules and the Surface Potentials of Their Monolayers	353
8.5. Applications to the Determination of Structure	358
References	368
9. Dipole Moments BY L. E. SUTTON	373
9.1. Introduction	373
9.2. The Theory and Practice of Measuring Electric Dipole Moments	376
9.3. Applications of Electric Dipole Moments to Simple Stereochemical Problems	382
9.4. Electric Dipole Moments and Electron Distribution	387
9.5. Applications of Electrical Dipole Moments to Complex Stereochemical Problems	400
9.6. Electric Dipole Moments and Molecular Interactions	413
9.7. Concluding Remarks	419
References	420
10. Electron Diffraction BY J. KARLE AND I. L. KARLE	427
10.1. Introduction	427
10.2. Instrumentation	429
10.3. The Theory of Electron Diffraction	431
10.4. The Analysis of Electron Diffraction Patterns	434
10.5. Applications to Organic Compounds	441
References	459
11. X-Ray Diffraction BY J. M. ROBERTSON	463
11.1. Principles of X-Ray Diffraction	463

11.2. The Phase Problem	469
11.3. Quantitative Measurements of Bond Lengths and Valency Angles in Known Structures	475
11.4. Applications to Unknown and Partially Unknown Structures	481
11.5. Intermolecular Interactions	493
References	499
12. Microwave Spectroscopy BY E. BRIGHT WILSON, JR., AND DAVID R. LIDE, JR.	503
12.1. Introduction	503
12.2. Principles of Rotational Spectra	503
12.3. Experimental Methods	507
12.4. Applications to the Determination of Structure	512
12.5. Individual Molecules	517
References	523
13. Thermodynamic Properties BY J. G. ASTON	525
13.1. Introduction	525
13.2. Thermodynamic Functions	525
13.3. Determination of Structure from Heat Capacity and Entropy	535
13.4. Aliphatic Hydrocarbons	544
13.5. Alicyclic Hydrocarbons	546
13.6. Functional Derivatives	551
13.7. Determination of Structure from Heats of Formation. Bond Energies and Resonance Energies	555
References	564
14. Dissociation Constants BY H. C. BROWN, D. H. McDANIEL, AND O. HÄFLIGER	567
14.1. Introduction	567
14.2. The Strengths of Protonic Acids and Bases	568
14.3. The Dissociation of Molecular Addition Compounds	634
14.4. The Application of Dissociation Constants to the Determination of the Structures of Natural Products and Related Compounds	643
References	655
15. Reaction Kinetics BY E. A. BRAUDE AND L. M. JACKMAN	663
15.1. Introduction	663
15.2. Principles of Reaction Kinetics	664
15.3. Determination of Electron Distribution	669
15.4. The Detection and Distinction of Structural Units	673
15.5. Determination of Stereochemical Configuration and Conformation	678
15.6. Investigation of Unstable Intermediates	696
15.7. Investigation of Inter- and Intra-molecular Complexes	715
References	719
16. Wave-Mechanical Theory BY C. A. COULSON	727
16.1. Introduction	727
16.2. Types of Bonds	728
16.3. Valence-Bond Treatment of Aromatic Systems	734
16.4. The Molecular-Orbital Method	746
References	756
AUTHOR INDEX	759
SUBJECT INDEX	783