CONTENTS

Preface v

1. LIQUID CRYSTALS AND MOLECULAR STRUCTURE - NEMATICS AND CHOLESTERICS 1

G.W. Gray

Introduction 1
Nematic (Cholesteric) Materials 5
Molecular Structural Features Common to many Nematogens 6
Lateral Substituents 14
Terminal Substituents 19
Cholesteric Liquid Crystals 26
Concluding Comments on Nematics/Cholesterics 27
References 28

2. INTERMOLECULAR FORCES 31

A.J. Stone

Introduction 31
Long-range Forces 33
Short-range Forces 40
Phenomenological Descriptions of the Intermolecular Potential 41
Description of Orientation Dependent Functions 43
References 49

3. DISTRIBUTION FUNCTIONS AND ORDER PARAMETERS 51

C. Zannoni

Introduction 51
Distributions 51
Thermodynamic Properties 56
Order Parameters 60
Molecular Symmetry and Mesophase Symmetry 64
Ordering Matrix 68
Smectics 70
Orientational Order Parameters for more Complex Phases 72
Pair Distribution 73
Nematics and Cholesterics 77
Appendix 78
References 83

CONTENTS

4. MOLECULAR FIELD THEORIES OF NEMATICS 85

G.R. Luckhurst

Introduction 85
The Molecular Field Approximation 86
The Maier-Saupe Theory of Nematics 91
Cylindrically Symmetric Molecules - the Complete Pair Potential 105
Non-cylindrically Symmetric Molecules 111
References 118

5. A MOLECULAR FIELD THEORY OF THE CHOLESTERIC LIQUID CRYSTAL STATE 121

H. Schröder

Introduction 121
The Intermolecular Potential 122
The Mean Field Approximation 132
Discussion of the Free Energy 133
Discussion of Phase Properties 136
References 146

6. A MOLECULAR MODEL FOR THE CHOLESTERIC MESOPHASE 149

B.W. van der Meer and G. Vertogen

Introduction 149
The Symmetry of the Chiral Interaction 154
The Interaction Model 155
The Free Energy of the Cholesteric State 159
Extensions of the Theory 160
Conclusions 163
Appendix 164
References 165
Postscript 166

7. HARD PARTICLE THEORIES OF NEMATICS 169

M.A. Cotter

Introduction 169
The Hard Rod Fluid 169
The Cluster Expansion Approach 171
The Scaled Particle Approach 174
Other Approaches 179
References 180

8. THE VAN DER WAALS APPROACH TO NEMATIC LIQUIDS 181

M.A.Cotter

Introduction 181
Statistical Mechanics 181
The Pseudo-potential $\bar{\psi}(\Omega,\rho)$ 183
Results 185
Discussion 188
References 189

CONTENTS

9. COMPUTER SIMULATIONS 191

C. Zannoni

Introduction 191
The Monte Carlo Method 193
Lattice Models 205
Molecular Dynamics 211
References 219

10. THERMODYNAMICS OF PHASE TRANSITIONS 221

D.E. Martire

Single Component Systems 221
Binary Mixtures 227
Appendix 236
References 236

11. STATISTICAL MECHANICS OF BINARY MIXTURES 239

D.E. Martire

Lattice Models 239
Molecular Field Theory 247
Comparison of all Theories with Experiment 256
References 261

12. LIQUID CRYSTALS AND MOLECULAR STRUCTURE-SMECTICS 263

G.W. Gray

Introduction 263
General Considerations 263
Considerations of Individual Smectic Polymorphic Types 268
Smectic A Phases 269
Smectic B Phases 270
Smectic E Phases 271
Molecular Structural Effects on S_A, S_B and S_E Phases 272
Smectic C Phases 274
Chiral S_C Phases 278
Smectic D Phases 279
Smectic F Phases 280
Smectic G Phases 280
Smectic H Phases 281
Chiral S_F, S_G and S_H Phases 282
Smectic Properties and Cholesteric Materials 282
References 283

13. STRUCTURAL STUDIES OF NEMATIC, SMECTIC A AND SMECTIC C PHASES 285

A.J. Leadbetter

Introduction 285
General Background 286
Application to Liquid Crystals. Descriptive Outline 296
Determination of the Distribution Function 306
References 315

14. X-RAY STUDIES OF ORDERED SMECTIC PHASES 317

J. Doucet

Introduction 317
Summary of X-ray Diffraction by Crystals 317
Liquid Crystal Phases 324
Study of the Ordered Smectic Phases of TBBA 325
Study of the S_B and S_E Phases of PBAPC 330
Study of Smectic F and Smectic G Phases 333
X-ray and Neutron Analysis of the Diffuse Spots located around the Bragg Spots (hko) 335
Diffraction by Mesogenic Crystals 338
Conclusion 340
Bibliography 340
References 341

15. NUCLEAR MAGNETIC RESONANCE STUDIES OF MOLECULAR BEHAVIOUR 343

J. Charvolin and B. Deloche

Introduction 343
Relevant Aspects of Magnetic Resonance 344
EPR of Spin Probes 349
Quadrupolar Effects in NMR 349
The Ordering Matrix 352
The Molecular Geometry 358
Motion and Analysis of the Results 362
Conclusion 364
References 365

16. MAGNETIC RESONANCE SPECTROSCOPY - STATIC BEHAVIOUR 367

P.L. Nordio and U. Segre

Introduction 367
Magnetic Interactions 368
Order Parameters 370
Orientational Distribution Function 373
Angular Dependence of the Magnetic Interactions 374
Spin Probes for Molecular Ordering 377
Experimental Applications 381
References 384

17. RAMAN STUDIES OF ORIENTATIONAL ORDER IN LIQUID CRYSTALS 385

P.S. Pershan

Introduction 385
Molecular Polarizability 385
Experimental Details 395
Measurements and Interpretation 401
Intrinsic Vibrations of MBBA 403
Final Remarks 409
References 410

CONTENTS

18. ROTATIONAL DYNAMICS 411

P.L. Nordio and U. Segre

Introduction 411
Stochastic Processes 411
Molecular Reorientation in Anisotropic Liquids 413
The Strong Collision Model 416
The Diffusion Model 417
Experimental Information on Orientational Time Correlation Functions 423
References 425

19. MAGNETIC RESONANCE SPECTROSCOPY - DYNAMICAL ASPECTS 427

P.L. Nordio and U. Segre

Relaxation and Lineshapes 427
Theory of Relaxation 431
Relaxation Mechanisms in Liquids 432
Spin Dynamical Variables 436
Kinetic Equations for the Dynamical Variables 440
Application to S=1 and S=3/2 Spin Systems 442
Determination of the Order Parameter $\bar{P}_4$ 446
Appendix 447
References 448

20. INCOHERENT QUASIELASTIC NEUTRON SCATTERING 451

A.J. Leadbetter and R.M. Richardson

General Aspects 451
Theory of Incoherent Quasielastic Neutron Scattering 453
Experimental Results 465
End Group Rotation in Solid Phases of Liquid Crystalline Systems 468
Summary of Experiments on Liquid Crystalline Phases 472
Conclusion 482
References 482

Subject Index 485

Chemical Index 493