

# CONTENTS

LIST OF CONTRIBUTORS TO PART III.....	v
PREFACE .....	vii
CONDENSED TABLE OF CONTENTS OF PARTS I-III .....	viii
Introduction, Parts I-III .....	1
<b>O. SINANOĞLU</b>	

## Section III. A. Light and Molecules

### 1. Interaction of Light with Matter and Theory of Optical Rotatory Power

**L. J. OOSTERHOFF**

1. Introduction .....	5
2. Propagation of Light in Transparent Matter .....	7
3. Propagation of Light in an Aggregate of Particles .....	9
4. Transition from Molecular Theory to Phenomenological Theory ....	11
5. Averaging over Physical Elements of Volume .....	13
6. Application to Averaging Maxwell's Microscopic Equations .....	15
7. Calculation of Induced Molecular Moments .....	19
8. Determination of the Internal Field .....	22
9. Statistical Derivation of the Wave Equation .....	25
10. Quantum Chemical Aspects .....	27
References .....	28

### 2. Two Theorems Useful for Optical Activity Calculations

**ALBERT MOSCOWITZ**

1. Introduction .....	31
2. Review of Pertinent Background Material .....	31
3. Proofs of Theorems I and II .....	34
4. Some Applications of Theorems I and II .....	38
References .....	43

### 3. Dipole Moments of Molecules in Excited States and the Effect of External Electric Fields on the Optical Absorption of Molecules in Solution

**WOLFGANG LIPTAY**

1. Introduction .....	45
2. The Average Transition Probability of a Molecule with a Definite Orientation .....	47
3. The Electric Field at the Location of a Molecule in Solution .....	49
4. The Wavenumber Shift $\Delta \tilde{\nu}_F$ .....	51
5. The Field Dependence of the Transition Moment .....	52
6. The Average Transition Probability of a Molecule in an Assembly in an Electric Field .....	53

7. Applications .....	57
Appendix. Calculation of the Average Transition Probability $\Pi\chi(\tilde{\nu}_F)$ .....	61
References .....	65
<b>4. Singlet-Triplet Intervals</b>	
<b>S. P. McGLYNN and F. J. SMITH</b>	
1. Introduction .....	67
2. Survey of Data .....	68
3. Conclusion .....	79
References .....	80
<b>5. Transition Moments and the Anisotropy of Fluorescence and Phosphorescence</b>	
<b>WOLFGANG LIPTAY</b>	
1. Introduction .....	81
2. Degree of Anisotropy of an Emission .....	83
3. Applications of the Degree of Anisotropy .....	86
4. Discussion .....	90
References .....	92
 <b>Section III. B. Light and Organic Crystals</b>	
<b>1. Delocalized Excitation and Excitation Transfer</b>	
<b>TH. FÖRSTER</b>	
1. Introduction .....	93
2. Formal Exciton Theory .....	95
3. Strong and Weak Coupling .....	105
4. Very Weak Coupling .....	120
5. Conclusions .....	136
References .....	137
<b>2. Excitons and Energy Transfer in Molecular Crystals</b>	
<b>JOSHUA JORTNER, STUART A. RICE, and ROBERT SILBEY</b>	
1. Introduction .....	139
2. Exciton Theory .....	141
3. Singlet Exciton States .....	145
4. Evaluation of the Matrix Elements .....	146
5. Long Range Interactions .....	150
6. Numerical Results for Singlet Exciton States of the Anthracene Crystal	152
7. Triplet Exciton States .....	156
8. Conclusions .....	159
References .....	159
<b>3. Coupling of the Molecular Exciton with the Nuclear Vibrations</b>	
<b>ANDRZEJ WITKOWSKI</b>	
1. Introduction .....	161
2. Monomer .....	162

3. Dimer .....	162
4. A Special Model: Bicycloheptadiene .....	164
5. The Potential Energy Curves .....	166
6. Perturbation Solution of Vibronic Equation: Strong Coupling .....	168
7. Intensities .....	170
8. Vibronic Equation for the Triplet Exciton .....	173
References .....	175
<b>4. Continuum Models and Dispersion Relations for Molecular Crystals</b>	
<b>A. T. AMOS</b>	
1. Introduction .....	177
2. The Basic Theory .....	177
3. The Electrostatic Model .....	179
4. Electromagnetic Solutions .....	181
5. Dispersion Relations .....	183
6. Conclusion .....	184
References .....	184
<b>5. Use of Green's Functions in the Theory of Excitons</b>	
<b>C. MAVROYANNIS</b>	
1. Introduction .....	185
2. Theory .....	185
3. Green's Functions and Energies of Excitation .....	191
4. Ground-State Energy .....	194
5. Appendix .....	198
References .....	201
<b>6. Interaction of Molecular Exciton, Charge Resonance States, and Excimer Luminescence</b>	
<b>S. P. McGLYNN, A. T. ARMSTRONG, and T. AZUMI</b>	
1. Introduction .....	203
2. Group Theoretic Considerations .....	204
3. Quantum Chemical Computations .....	210
4. Conclusions .....	227
5. Summary .....	228
References .....	228
<b>7. Electronic Excitations in Molecules with Transannular Interactions</b>	
<b>J. KOUTECKÝ and J. PALDUS</b>	
Text .....	229
References .....	233
<b>8. Photoconductivity in Crystals of Organic Molecules</b>	
<b>JOSHUA JORTNER and STUART A. RICE</b>	
1. Introduction .....	235
2. The Energy Balance Problem .....	236

3. The Auger Effect for a Pair of Excited Hydrogen Atoms .....	238
4. Exciton-Exciton Interactions in the Anthracene Crystal .....	240
5. The Exciton-Photon Interaction .....	244
6. Charge Carrier Mobility in Organic Crystals .....	246
References .....	248
<b>9. Temperature Dependence of Photoconductivity in Organic Molecular Crystals</b>	
<b>S. P. McGLYNN, L. AZARRAGA, and F. WATSON</b>	
1. Introduction .....	249
2. Thermal Activation Energy of Photoconductivity .....	249
References .....	255
<b>10. Laser Generation and Transport Properties of Triplet Excitons in Anthracene Crystals</b>	
<b>W. SIEBRAND</b>	
1. Introduction .....	257
2. Triplet Exciton Generation Processes .....	259
3. Properties of Triplet Excitons .....	260
References .....	263
<b>11. Surface and Impurity States in Crystals</b>	
<b>A. T. AMOS</b>	
1. Introduction .....	265
2. Tamm Surface States .....	266
3. Shockley States .....	268
4. Localized Impurity States .....	269
5. The Dynamical Problem .....	272
References .....	273
<b>12. Interpretation of Surface States of Electrons in Crystals</b>	
<b>J. KOUTECKÝ</b>	
Text .....	275
References .....	280
<b>13. Hydrogen Bonding and Energy Bands in Proteins</b>	
<b>ALBERTE PULLMAN</b>	
1. Introduction .....	283
2. The Evans and Gergely Calculation .....	286
3. The Points Calling for Discussion .....	288
4. The Theoretical Treatment of Suard, Berthier, and Pullman .....	291
5. Other Calculations .....	307
References .....	310
<b>AUTHOR INDEX</b> .....	313
<b>SUBJECT INDEX</b> .....	319