

Contents

1. THE DYNAMICS OF MOLECULAR COLLISIONS	1
1.1. What is molecular dynamics?	1
1.2. An example: infrared chemiluminescence	1
1.3. Why molecular dynamics?	4
1.4. A simple model of energy partitioning	7
1.5. The need to know	11
Appendix 1A: What are the new techniques?	14
2. MOLECULAR COLLISIONS	16
2.1. Molecular collisions and free path phenomena	16
Appendix 2A: Transport coefficients	21
2.2. Collision cross-sections and the intermolecular potential	22
2.3. Dynamics of elastic molecular collisions	27
2.4. The reaction cross-section	35
2.5. The reaction probability	40
Suggested readings	47
3. SCATTERING AS A PROBE OF THE COLLISION DYNAMICS	49
3.1. Elastic scattering as a probe of the interaction potential	49
Appendix 3A: Relation between scattering in the c.m. and laboratory system	60
3.2. Intermolecular potentials from experiment and theory	63
3.3. Angular distribution in direct reactive collisions	69
Suggested readings	77
4. THE POLYATOMIC APPROACH TO CHEMICAL DYNAMICS	78
4.1. Three-body potential energy functions and chemical reactions	78
4.2. The classical trajectory approach to reaction dynamics	90
Appendix 4A: Mass-weighted co-ordinate systems	98
4.3. Theoretical approaches to the overall reaction rate	100
4.4. From microscopic dynamics to macroscopic kinetics	108
4.5. Energy and chemical change	114
Suggested readings	122
5. MOLECULAR ENERGY TRANSFER	125
5.1. A macroscopic description of energy transfer	125
5.2. Time resolved spectroscopy: The CO ₂ laser	129
5.3. Simple models of energy transfer	135
5.4. Rotational energy transfer	143
5.5. The role of intermolecular potentials in energy transfer	148

5.6. Inelastic collision theory	154
5.7. Bimolecular spectroscopy	162
5.8. Electronic energy transfer	168
Suggested readings	179
6. REACTION DYNAMICS	181
6.1. Experimental methods in molecular reaction dynamics	181
6.2. The collisional method	191
6.3. A case study of a well-characterized elementary reaction	203
Appendix 6A: Role of angular momentum in reactive collisions	211
6.4. Collision complexes: Their formation and decay	213
Appendix 6B: A statistical theory of complex formation and decay	224
6.5. The road ahead	227
Suggested readings	233
GENERAL APPENDIX	235
1. Table of useful physical constants	235
2. Table of useful conversion factors	235
3. Table of (approximate) energy conversion factors	236
AUTHOR INDEX	238
SUBJECT INDEX	240