## Contents

1	New	Ideas for Solving Old Problems - An Introduction	1
Pa	rt I (	Group Theory in Molecular Physics	
2	Basi	c Concepts	9
	2.1	Symmetry Groups of the Molecular Hamiltonian	9
		2.1.1 General Representation Theory	11
		2.1.2 Lie Groups and Permutation Groups	14
	2.2	Zero-Order Models in Molecular Theory	18
		2.2.1 The Separation of the Molecular Hamiltonian	19
		2.2.2 The Zero-Order Models for Nuclear Motion	22
	2.3	Connecting Dynamics and Group Theory – Outlook	
		to This Work	25
3	Schu	r–Weyl Duality in Molecules	27
	3.1	Nuclear Spin States in Molecules	27
		3.1.1 The Natural Way	31
		3.1.2 Unitary Symmetry	35
		3.1.3 Permutation Symmetry	37
	3.2	Schur–Weyl Duality	39
		3.2.1 Application of the Duality Theorem	40
	3.3	Conclusion	41
4	Read	tive Collisions	45
	4.1	Representation Theory in Reactions of Small Molecules	47
		4.1.1 Mathematical Preliminaries	47
		4.1.2 Single Molecules	49
		4.1.3 A First Example	51

Contents

4.2	The $H_3^+$ + $H_2$ Reaction	53
	4.2.1 A Restricted Symmetry Group for the Intermediate	
	Complex	56
	4.2.2 Implications for Experiments	59
	4.2.3 The Deuterated Version	59
4.3	Discussion	62

## Part II Extremely Floppy Molecules

5	Intro	ducing Extreme Floppiness	67
6	<b>Symn</b> 6.1 6.2 6.3	netry Beyond Perturbation TheoryRepresentation Theory of Molecular Rotation. $6.1.1$ Example: The $H_3^+$ ionThe Failure of the Subgroup Picture.Concluding Remarks.	71 71 81 82 86
7	<b>The N</b> 7.1 7.2	Molecular Super-RotorLarge Amplitude MotionSuper-Rotation7.2.1The Energy Expression7.2.2Degrees of Freedom	87 87 91 93 94
8	Super 8.1 8.2 8.3	r-Rotor States and Their Symmetry.    Five-Dimensional Rotor States    8.1.1  Parity and Dipole Selection Rules    Permutation-Inversion Symmetry    8.2.1  The Permutation Group of Five Identical Particles    Conclusion	95 95 99 100 102 105
9	<b>Proto</b> 9.1 9.2 9.3 9.4	nated MethaneThe MoleculeThe ExperimentThe ModelThe Discussion	107 107 109 111 115
10	<b>Refin</b> 10.1 10.2 10.3	ements and Further Applications.Beyond Zero-Order.10.1.1Generalized Moments of Inertia.10.1.2Higher-Order TermsAdditional Target Molecules.Concluding Remarks.	117 117 117 120 121 123

Contents

## Part III Semi-classical Approach to Rotational Dynamics

11	Ultra	fast Rotation	127	
	11.1	Introduction	127	
	11.2	The Gutzwiller Trace Formula	129	
	11.3	The Rotational Energy Surface	136	
		11.3.1 The Paths on the Rotational Energy Surface	139	
		11.3.2 The Quantization Conditions	142	
		11.3.3 Two Approaches to Generate the Rotational Energy		
		Surface	144	
12	Appli	ication to Sulfur Dioxide	149	
	12.1	The Molecule	149	
	12.2	The Comparison	150	
13	Discu	ission	155	
	13.1	The TROVE - Generated Rotational Energy Surface	155	
	13.2	Generalization of the Approach	156	
14	New	Ideas for Solving Old Problems – A Conclusion	159	
Ref	erence	s	163	
Index				