



CONTENTS

ANGULAR DISTRIBUTIONS OF PHOTOELECTRONS: CONSEQUENCES OF SYMMETRY

By Murray Peshkin 1

ELECTRON-IMPACT SPECTROMETRY

By Sandor Trajmar, James K. Rice, and Aron Kuppermann 15

MODELS, INTERPRETATIONS, AND CALCULATIONS CONCERNING RESONANT ELECTRON SCATTERING PROCESSES IN ATOMS AND MOLECULES

By Howard S. Taylor 91

ELECTRON RESONANCE OF GASEOUS DIATOMIC MOLECULES

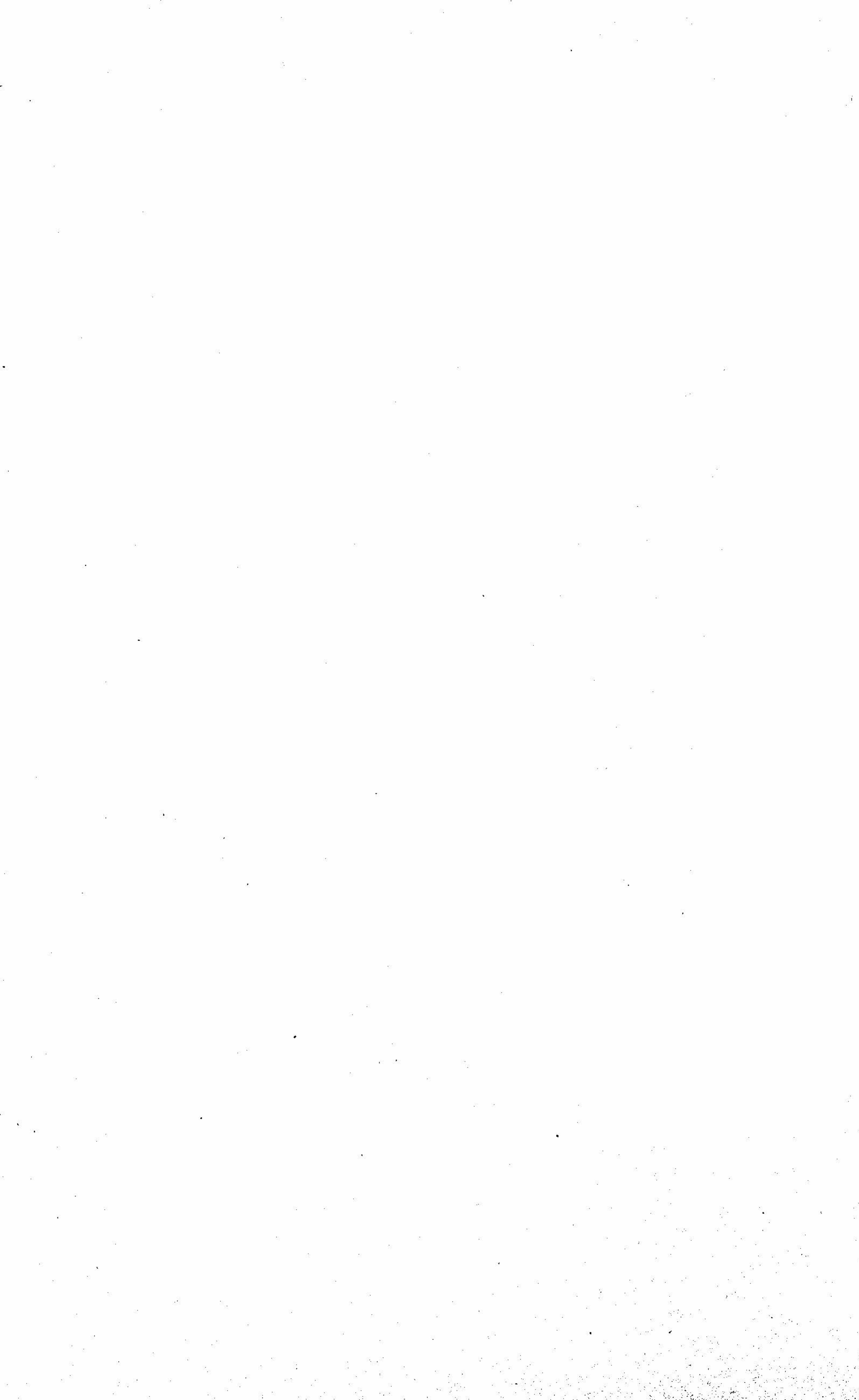
By Alan Carrington, Donald H. Levy, and Terry A. Miller 149

APPROXIMATE MOLECULAR ORBITAL THEORIES

By B. J. Nicholson 249

AUTHOR INDEX 313

SUBJECT INDEX 319



ANGULAR DISTRIBUTIONS OF PHOTOELECTRONS: CONSEQUENCES OF SYMMETRY

MURRAY PESHKIN*

*The Weizmann Institute of Science, Rehovot, Israel, and
Argonne National Laboratory, Argonne, Illinois*

CONTENTS

I. Introduction and Conclusions	1
II. Polarization States of a Photon	2
III. Multipole Decomposition	5
IV. The Photon Density Matrix	6
V. Expansion in Standard Tensors	8
VI. Angular Distribution of One Electron	10
VII. Two-Electron Angular Distributions	13
References	14

ELECTRON-IMPACT SPECTROMETRY

SANDOR TRAJMAR,*† JAMES K. RICE,† AND
ARON KUPPERMANN†

*California Institute of Technology
Pasadena, California*

CONTENTS

I. Introduction	15
II. Historical Development	19
III. Experimental	21
A. Pressure Dependence	24
B. Effective Path Length Correction	26
C. Energy Independent Electron Optics	26
VI. Electronic Excitation	27
A. Helium	30
B. Molecules	41
1. Nitrogen	42
2. Carbon Monoxide	48
3. Hydrogen	51
4. Acetylene	56
5. Ethylene	61
C. Summary	67
V. Vibrational-Rotational Excitation	70
VI. Superelastic Scattering	83
VII. Positron Scattering	86
References	86

MODELS, INTERPRETATIONS, AND CALCULATIONS CONCERNING RESONANT ELECTRON SCATTERING PROCESSES IN ATOMS AND MOLECULES

HOWARD S. TAYLOR*

*Department of Chemistry
University of Southern California
Los Angeles, California*

CONTENTS

I.	Mechanistic Model for Resonances	92
II.	The Stabilization Method	100
A.	Introduction	100
B.	Heuristic Approaches	102
C.	A Suggestive and Related Problem	105
D.	Comment on the Mathematical Description of Resonances	110
III.	Application of the Models and the Stabilization Method	115
A.	The Angular Dependence in the Vibrational Excitation Process in N_2 , CO, and H_2	115
B.	Resonant Phenomena in the Hydrogen Molecule	124
C.	Use of the One-Electron Model in the Qualitative Understanding and Choices of Significant Experiments	140
D.	Resonant Scattering for the Helium Atom	144
	References	145

ELECTRON RESONANCE OF GASEOUS DIATOMIC MOLECULES

ALAN CARRINGTON

*Department of Chemistry, University of Southampton,
Southampton, England*

DONALD H. LEVY*

*Department of Chemistry and the James Franck Institute,
University of Chicago, Chicago, Illinois*

and

TERRY A. MILLER

Bell Telephone Laboratories, Inc., Murray Hill, New Jersey

CONTENTS

I. Introduction	150
II. Derivation of the Hamiltonian	151
A. Foundations of the Derivation	151
B. Separation of Nuclear and Electronic Motion	156
C. Derivation of the Clamped Nuclei Hamiltonian	167
III. Calculation of the Matrix Elements	183
A. Important Results from the Theory of Angular Momentum	183
B. Matrix Elements in Hund's Case (a)	187
1. Purely Rotational Hamiltonian	187
2. Spin-Rotation Interaction	190
3. Fine-Structure Hamiltonian	193
4. Nuclear Magnetic and Electric Hyperfine Structure	195
5. Interaction with the External Magnetic Field	200
C. Matrix Elements in Hund's Case (b)	202
1. Fine-Structure Hamiltonian	202
2. Rotationally-Dependent Interactions	203
3. External Magnetic Field Interactions	205
4. Nuclear Magnetic and Electric Hyperfine Structure	207

* Alfred P. Sloan Fellow.

IV. Interpretation of Electron Resonance Spectra	209
A. Rotational Energy Levels	209
B. Λ -Doubling	223
C. Nuclear Magnetic and Electric Hyperfine Couplings	227
D. Intensities and Lineshape	233
E. Stark Effect	237
V. Experimental	242
References	246

APPROXIMATE MOLECULAR ORBITAL THEORIES

B. J. NICHOLSON

*Trinity College,
Cambridge,
England*

CONTENTS

I. Introduction	249
II. Theoretical Background	251
III. Possible Approximations	253
A. The Mulliken Approximation	253
1. General Discussion	253
2. Preliminary Investigation	256
3. Errors in the Diagonal F-Matrix Elements	258
4. Errors in the Two-Center Off-Diagonal Elements	260
5. Final Remarks	265
B. The Ruedenberg Approximation	266
C. The Zero Differential Overlap Approximation	269
1. Preliminary Discussion	269
2. Numerical Investigation	271
D. Neglect of Inner Shells	277
E. Averaging for Rotational Invariance	281
F. Semiempirical Approximations	285
IV. Current Theories	289
A. Using the Mulliken Approximation	289
B. Using the Mulliken and Ruedenberg Approximations	290
C. Using the Zero Differential Overlap Approximation	291
V. Present Proposals	295
A. Formulation	295
B. Calibration	298
C. Reproduction of Reference Calculations	300
D. Agreement with Experiment	302
VI. Conclusions	305
References	305