
Contents

Foreword	vii
Editors	xi
Contributors	xiii
Introduction	xv
Principal Structures	xix
Chapter 1 Quantum Theory of Equilibrium Molecular Structures	1
<i>Wesley D. Allen and Attila G. Császár</i>	
Chapter 2 The Method of Least Squares	29
<i>Jean Demaison</i>	
Chapter 3 Semiexperimental Equilibrium Structures: Computational Aspects	53
<i>Juana Vázquez and John F. Stanton</i>	
Chapter 4 Spectroscopy of Polyatomic Molecules: Determination of the Rotational Constants	89
<i>Agnès Perrin, Jean Demaison, Jean-Marie Flaud, Walter J. Lafferty, and Kamil Sarka</i>	
Chapter 5 Determination of the Structural Parameters from the Inertial Moments	125
<i>Heinz Dieter Rudolph and Jean Demaison</i>	
Chapter 6 Determining Equilibrium Structures and Potential Energy Functions for Diatomic Molecules	159
<i>Robert J. Le Roy</i>	
Chapter 7 Other Spectroscopic Sources of Molecular Properties: Intermolecular Complexes as Examples	205
<i>Anthony C. Legon and Jean Demaison</i>	

Chapter 8 Structures Averaged over Nuclear Motions	233
<i>Attila G. Császár</i>	
Appendix A: Bibliographies of Equilibrium Structures	263
Appendix B: Sources for Fundamental Constants, Conversion Factors, and Atomic and Nuclear Masses	265
Author Index	267
Subject Index	275