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Titolo	Global and accurate vibration Hamiltonians from high resolution molecular spectroscopy [[electronic resource] /] / edited by Michel Herman ... [et al.]
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Nota di contenuto	Advances in CHEMICAL PHYSICS; CONTENTS; Series Introduction; I. General Introduction; II. The Forward Trip: From the Hamiltonian to the Vibration-Rotation Spectrum; A. Introduction; B. The Forward Trip: An Ab Initio Approach; 1. Exact Quantum Mechanical Formulation; a. Full Molecular Hamiltonian; b. Born-Oppenheimer Separation; c. Translation-Free Hamiltonian; d. Vibration-Rotation Separation; 1. MOLECULAR AXIS SYSTEM (MAS); 2. ROTATION COORDINATES; 3. ECKART FRAME; 4. VIBRATION COORDINATES; e. Exact Vibration-Rotation Hamiltonian; 1. VIBRATION-ROTATION KINETIC ENERGY OPERATOR 2. POTENTIAL-ENERGY SURFACE3. EXACT VIBRATION-ROTATION SCHRODINGER EQUATION; f. Variational Resolution of the Vibration-Rotation Schrodinger equation; 1. VARIATIONAL PRINCIPLE; 2. LINEAR VARIATIONAL METHOD; 3. CONFIGURATION INTERACTION METHOD; 4.

DIAGONALISATION OF THE VIBRATION-ROTATION HAMILTONIAN; 5. ENERGY SPECTRUM OF THE VIBRATION-ROTATION HAMILTONIAN; 6. VIBRATION-ROTATION TRANSITION ENERGIES; g. Vibration-Rotation Lines Intensities; 1 . OPTICAL VIBRATION-ROTATION TRANSITION PROBABILITIES; 2. ELECTRIC DIPOLE TRANSITION PROBABILITIES; 3. DIPOLE MOMENT SURFACE
h. Full Ab Inirio Forward Trip2. Towards a Converged Ab Initio Approach; a. Setting the Ab Initio Approach; 1. NEED FOR A PES; 2. GENERAL PROBLEMS WITH PES AND DMS; b. Choice of a Coordinate System; 1. CRITERIA; 2. RECTILINEAR VERSUS CURVILINEAR COORDINATES; c. Selected Curvilinear Coordinates; 1. CURVILINEAR BOND-ANGLE COORDINATES; 2. LOCAL-MODE COORDINATES; 3. HELIOCENTRIC-TYPE COORDINATES; 4. ADAPTED STRETCHING COORDINATES; 5. POTENTIAL-ADAPTED COORDINATES; 6. ADAPTED BENDING COORDINATES; 7. OPTIMISED COORDINATES; 8. CURVILINEAR NORMAL COORDINATES; 9. TRANSFORMATION OF COORDINATES
d. Approximate PES from Quantum Chemistry1. AB INITIO LEVEL OF CALCULATION; 2. ANALYTICAL EXPRESSION FOR THE PES; 3. ADJUSTMENT OF AN ANALYTICAL FUNCTION TO AB INITIO CALCULATED POINTS; 4. ANALYTICAL VERSUS NUMERICAL DERIVATIVES CALCULATIONS; 5. AB INITIO DVR APPROACH; e. Ah initio Electric Dipole Moment Surfaces; f. Variational Methods; 1. CONTRACTION OR DIAGONALIZATION-TRUNCATION; 2. GENERAL MEAN-FIELD OPTIMIZATIONS; 3. THE VIBRATIONAL MULTICONFIGURATIONAL SCF METHOD; 4. DISCRETE-VARIABLE REPRESENTATION (DVR); 5. ADIABATIC APPROACHES
6. MORSE OSCILLATOR RIGID BENDER INTERNAL DYNAMICS (MORBID) APPROACHg. Perturbation Theory Methods; 1. BASIC FORMULAS; 2. TREATMENT OF RESONATING STATES; 3. HIGH ORDER CANONICAL VAN VLECK PERTURBATION THEORY (CVPT); C. Acetylene: A Laboratory for Intramolecular Advances; 1. The Acetylene Molecule; a. Both Simple and Complex; b. Symmetry Properties; c. Topology of the Ground-State PES; d. Calculated Properties; e. Coordinate Systems; 1. 9D SYSTEMS; 2. 6D SYSTEMS; 3. SYMMETRY-ADAPTED COORDINATES; 4. RECTILINEAR NORMAL COORDINATES; 5. PLANAR 5D SYSTEMS
f. Vibration-Rotation Hamiltonian for Acetylene

Sommario/riassunto

The latest in a series providing chemical physicists with a forum for critical, authoritative evaluations of advances in every area of the discipline, this stand-alone volume focuses on using high resolution molecular spectroscopy to arrive at global and accurate Vibration Hamiltonians.

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Autore	Pepper Darrell W
Titolo	Modeling indoor air pollution / / Darrell W. Pepper, David Carrington
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Nota di contenuto	Acknowledgements; Preface; Contents; 1. Introduction; 2. Fluid Flow Fundamentals; 3. Contaminant Sources; 4. Assessment Criteria; 5. Simple Modeling Techniques; 6. Dynamics of Particles, Gases and Vapors; 7. Numerical Modeling - Conventional Techniques; 8. Numerical Modeling - Advanced Techniques; 9. Turbulence Modeling; 10. Homeland Security Issues; Appendix A Diffusion Coefficients in Gas; Appendix B 2-D Office Simulations: COMSOL and ANSWER Software; Bibliography; Index
Sommario/riassunto	Emission of pollutants and their accumulation due to poor ventilation and air exchange are serious problems currently under investigation by many researchers. Of particular concern are issues involving air quality within buildings. Toxic fumes and airborne diseases are known to produce undesirable odors, eye and nose irritations, sickness, and occasionally death. Other products such as tobacco smoke and carbon monoxide can also have serious health effects on people exposed to a

poorly ventilated environment; studies indicate that indirect or passive smoking can also lead to lung cancer.Design