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Titolo	Global and accurate vibration Hamiltonians from high resolution molecular spectroscopy / / edited by Michel Herman ... [et al.]
Pubbl/distr/stampa	New York ; ; Chichester, : Wiley, c1999
ISBN	9786612682025 9781282682023 1282682024 9780470141670 0470141670 9780470142202 0470142200
Descrizione fisica	1 online resource (450 p.)
Collana	Advances in chemical physics ; ; v. 108
Altri autori (Persone)	HermanMichel
Disciplina	541.3 541.305 541/.08
Soggetti	Hamiltonian systems Molecular spectroscopy High resolution spectroscopy

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Nota di bibliografia	Includes bibliographical references and indexes.
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.