

QUANTUM SYSTEMS IN
CHEMISTRY AND PHYSICS.
TRENDS IN METHODS
AND APPLICATIONS

edited by

Roy McWeeny, Jean Maruani, Yves G. Smeyers

and

Stephen Wilson



KLUWER ACADEMIC PUBLISHERS

DORDRECHT / BOSTON / LONDON

Table of Contents*

Preface	vii
* Introduction by ROY McWEENY / The European Workshop "Quantum Systems in Chemistry and Physics"	1
I) TRENDS IN METHODS	
* R. McWEENY / Separability in Quantum Mechanics	7
* T. GRABO, T. KREIBICH and E.K.U. GROSS / Optimized Effective Potential for Atoms and Molecules	27
* I. MARTIN / The Relativistic Quantum Defect Orbital Method and Some of its Applications	51
* T. THORSTEINSSON, D.L. COOPER, J. GERRATT and M. RAIMONDI / A New Approach for Valence-bond Calculations: CASVB	67
* M.A.C. NASCIMENTO / Studies on Chemical Structure, Spectroscopy and Electron Scattering Using Generalized Multistructural Wavefunctions	87
II) TRENDS IN APPLICATIONS	
* S.G. CHRISTOV / The Characteristic (Crossover) Temperature in the Theory of Thermally Activated Tunneling Processes	109
* L. MIHAILOV, M. KIRTICHEVA and A. MANOV / An Improved method of Relaxation Rate Calculation in Double-well Potential Systems	149
* H. CHOJNACKI / Correlation Effects in the Double Proton Transfer of the Formic Acid Dimer	161
* I. ROSENBLUM, E.I. DASHEVSKAYA, E.E. NIKITIN and I. OREF / Effect of the Vibrational/Rotational Energy Partitioning on the Energy Transfer in Atom-triatomic Molecule Collisions	169

* Contributions indicated with an asterisk also appear in the journal *Molecular Engineering*, Volume 7, Nos. 1-2.

* E. BUONOMO and F.A. GIANTURCO / Fragmentation of Ar_3^+ : the Role of Rotational and Vibrational Predissociation Dynamics	185
* G. DELGADO-BARRIO, A. GARCIA-VELA, C. GARCIA-RIZO, M.I. HERNANDEZ and P. VILLAREAL / Sampling the Initial Conditions for Quasi-classical Trajectory Studies of Vibrational Predissociation Dynamics	219
* C. PISANI and S. CASASSA / Energy Estimates for Local Chemical Processes in Condensed Matter	231
* A. MARKOVITS, J. AHDJOU DJ and C. MINOT / Theoretical Study of the TiO_2 and MgO Surface Acidity and the Adsorption of Acids and Bases	245
* M. GEORGIEV and L. MIHAILOV / Optical Spectra of High-temperature Superconductors	263
III) ADDITIONAL CONTRIBUTIONS	
J. MASIK and I. HUBAC / Multireference Brillouin–Wigner Coupled-Cluster Theory: Hilbert Space Approach	283
L.S. GEORGIEV, YA.I. DELCHEV, R.L. PAVLOV and J. MARUANI / Core-Valence Separation for an Open-shell Atom in the LST-DFT Scheme	309
D. MONCRIEFF and S. WILSON / On the Accuracy of the Algebraic Approximation in Molecular Electronic Structure Studies: Matrix Valence-bond Calculations for the Hydrogen Molecule Ground State	323
C. AMOVILLI / On the Evaluation of the Matrix Elements Between Non-Orthogonal Slater Determinants	343
R. MOCCIA, S. MENGALI and R. MONTUORO / The Calculation of Some Processes Involving Transitions in the Continuum	349
M. IVANOVITCH, M. GEORGIEV, M. MLADENOVA, G. BALDACCHINI, R.M. MONTEREALI, U.M. GRASSANO and A. SCACCO / Revisiting the Off-center Impurity Problem: Reorientational Rates of Hindered Rotators	373
Subject Index	397