

Contents

Preface to the special collection in honor of Gregory S. Ezra	1
Srihari Keshavamurthy, Stephen Wiggins	
Roaming dynamics in ketene isomerization	11
Frédéric A. L. Mauguière, Peter Collins, Gregory S. Ezra, Stavros C. Farantos, Stephen Wiggins	
Revisiting roaming trajectories in ketene isomerization at higher dimensionality	25
Inga S. Ulusoy, Rigoberto Hernandez	
Toward a quantum trajectory-based rate theory	35
Brittany L. Hyland, Craig C. Martens	
Semiclassical quantization of atomic systems through their normal form: the hydrogen atom	45
Charles Jaffé, Jesús Palacián, Patricia Yanguas, T. Uzer	
A semiclassical adiabatic calculation of state densities for molecules exhibiting torsion: application to hydrogen peroxide and its isotopomers	53
Zeb C. Kramer, Rex T. Skodje	
The semiclassical propagator in fermionic Fock space	67
Thomas Engl, Peter Plöchl, Juan Diego Urbina, Klaus Richter	
A new method to improve validity range of Lie canonical perturbation theory: with a central focus on a concept of non-blow-up region	89
Hiroshi Teramoto, Mikito Toda, Tamiki Komatsuzaki	
Signatures of classical bifurcations in the quantum scattering resonances of dissociating molecules	105
Pierre Gaspard	
Topological phase transitions in the vibration–rotation dynamics of an isolated molecule	115
T. Iwai, B. Zhilinskii	
Vibrational energy flow across heme–cytochrome <i>c</i> and cytochrome <i>c</i>–water interfaces	129
Johnson K. Agbo, Yao Xu, Ping Zhang, John E. Straub, David M. Leitner	
Quantum molecular dynamics simulations of liquid benzene using orbital optimization	139
Nazar Ileri, Laurence E. Fried	
Effect of a chiral electrostatic cavity on product selection in a reaction with a bifurcating reaction path	151
Barry K. Carpenter	
Computer simulation of quantum dynamics in a classical spin environment	159
Alessandro Sergi	
Ions in liquid metal clusters	175
R. Stephen Berry, Boris M. Smirnov	

Gregory S. Ezra

A Festschrift from Theoretical Chemistry Accounts

Keshavamurthy, S.; Wiggins, S. (Eds.)

2015, V, 183 p. 77 illus., 61 illus. in color., Hardcover

ISBN: 978-3-662-47376-4