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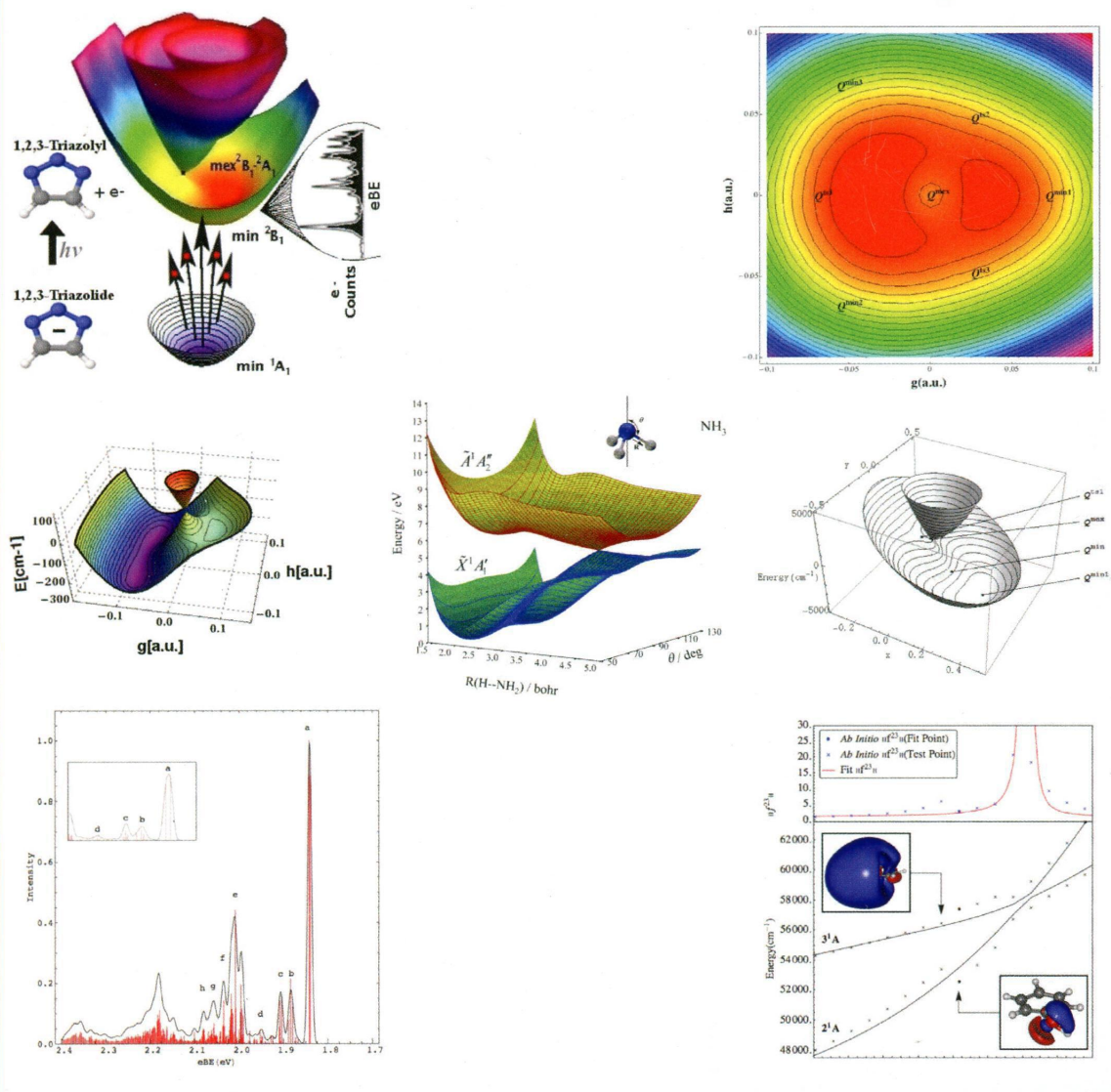
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THE JOURNAL OF PHYSICAL CHEMISTRY

A

DAVID R. YARKONY
FESTSCHRIFT

Nonadiabatic Processes:
Simulated Spectra,
Computational
Issues, and Conical
Intersections
Involving Triazolyl
and Isopropoxy;
Ethoxy, Ammonia,
and Pyrrolyl;
and Isopropoxy
and Phenol



ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY



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ON THE COVER: We have developed procedures for representing adiabatic potential energy surfaces coupled by conical intersections. These representations are achieved using demonstrably quasi diabatic electronic states. On the cover are pictured simulated spectra, computational issues, and conical intersections relevant to these coupled potential energy surfaces. Conically intersecting adiabatic potential energy surfaces for ethoxy [188], ammonia [212], and pyrrolyl [186] (middle row); the simulation of the negative ion photoelectron spectra of triazolyl [197] (top left) and isopropoxy [187] (bottom left); a slice through the gh plane of the lower adiabatic potential energy surface of isopropoxy [187] (top right), showing the minimum energy conical intersection, three minima, and three saddle points positioned surprisingly like those in a molecule with C_{3v} symmetry; and finally a figure [211] illustrating how our fitting procedure can smooth out irregularities in the electronic structure data resulting from changes in the active space orbitals that inevitably plague the ab initio data used to construct coupled global potential energy surfaces (bottom right). Numbers in square brackets refer to the papers listed in the “Publications of David R. Yarkony” (pp 11844–11851 in this issue). This special section was organized by Guest Editors Spiridoula Matsika, Henry F. Schaefer III, and Michael Schuurman.

SPECIAL SECTION: DAVID R. YARKONY FESTSCHRIFT

Guest Editors: Spiridoula Matsika, Henry F. Schaefer III, and Michael Schuurman


Special Issue Preface

- | | |
|--|------------------------|
| 11837
Tribute to David R. Yarkony
Spiridoula Matsika,* Henry F. Schaefer III, and Michael S. Schuurman | DOI: 10.1021/jp512064b |
| 11838
Autobiography of David R. Yarkony: My Life as a Scientist | DOI: 10.1021/jp5106357 |
| 11842
Collaborators of David R. Yarkony | DOI: 10.1021/jp510636a |
| 11843
Curriculum Vitae of David R. Yarkony | DOI: 10.1021/jp5106373 |
| 11844
Publications of David R. Yarkony | DOI: 10.1021/jp510638g |

Articles

- | | |
|---|------------------------|
| 11852
Jet-Cooled Laser-Induced Fluorescence Spectroscopy of Isopropoxy Radical: Vibronic Analysis of $\tilde{B}-\tilde{X}$ and $\tilde{B}-\tilde{A}$ Band Systems
Rabi Chhantyal-Pun, Mourad Roudjane, Dmitry G. Melnik, Terry A. Miller,* and Jinjun Liu | DOI: 10.1021/jp504322j |
|---|------------------------|


- 11871  DOI: 10.1021/jp504326p
Jet-Cooled Laser-Induced Fluorescence Spectroscopy of Cyclohexoxy: Rotational and Fine Structure of Molecules in Nearly Degenerate Electronic States
Jinjun Liu and Terry A. Miller*
-
- 11891 DOI: 10.1021/jp411107k
Analysis of Localized Diabatic States beyond the Condon Approximation for Excitation Energy Transfer Processes
Ethan C. Alguire, Shervin Fatehi, Yihan Shao, and Joseph E. Subotnik*
-
- 11901  DOI: 10.1021/jp504724v
Photoelectron Spectroscopic and Computational Study of Hydrated Pyrimidine Anions
John T. Kelly, Shoujun Xu, Jacob Graham, J. Michael Nilles, Dunja Radisic, Angela M. Buonaugurio, Kit H. Bowen Jr., Nathan I. Hammer,* and Gregory S. Tschumper*
-
- 11908 DOI: 10.1021/jp504889e
Influence of Light-Induced Conical Intersection on the Photodissociation Dynamics of D_2^+ Starting from Individual Vibrational Levels
Gábor J. Halász, András Csehi, Ágnes Vibók,* and Lorenz S. Cederbaum
-
- 11916  DOI: 10.1021/jp505108k
Imaging Studies of Excited and Dissociative States of Hydroxymethylene Produced in the Photodissociation of the Hydroxymethyl Radical
Chirantha P. Rodrigo, Subhasish Sutradhar, and Hanna Reisler*
-
- 11926 DOI: 10.1021/jp5057122
Full-Dimensional Quantum Dynamics of Vibrationally Mediated Photodissociation of NH_3 and ND_3 on Coupled Ab Initio Potential Energy Surfaces: Absorption Spectra and $NH_2(\tilde{A}^2A_1)/NH_2(\tilde{X}^2B_1)$ Branching Ratios
Jianyí Ma,* Changjian Xie, Xiaolei Zhu, David R. Yarkony,* Daiqian Xie,* and Hua Guo*
-
- 11935 DOI: 10.1021/jp505769h
Transport Properties for Systems with Deep Potential Wells: $H + O_2$
Paul J. Dagdigan* and Millard H. Alexander
-
- 11943  DOI: 10.1021/jp506090g
What We Can Learn from the Norms of One-Particle Density Matrices, and What We Can't: Some Results for Interstate Properties in Model Singlet Fission Systems
Spiridoula Matsika, Xintian Feng, Anatoliy V. Luzanov, and Anna I. Krylov*
-
- 11956 DOI: 10.1021/jp506287z
Surprising Quenching of the Spin–Orbit Interaction Significantly Diminishes $H_2O \cdots X$ [$X = F, Cl, Br, I$] Dissociation Energies
Gábor Czakó,* Attila G. Császár,* and Henry F. Schaefer III


11962  DOI: 10.1021/jp506793z
The $(E + A) \times (e + a)$ Jahn–Teller and Pseudo-Jahn–Teller Hamiltonian Including Spin–Orbit Coupling for Trigonal Systems
Swarnendu Bhattacharyya,* Daniel Opalka, Leonid V. Poluyanov, and Wolfgang Domcke*


11971 DOI: 10.1021/jp5070159
Two-Center Noninteger- n Overlap, Coulomb, and Kinetic Energy Integrals by Numerical Contour Integration
Harris J. Silverstone*


11975 DOI: 10.1021/jp507075c
Conformer-Resolved Quantum Dynamics Study of the Photodissociation of 3-Pyrroline
S. P. Neville and G. A. Worth*


11987 DOI: 10.1021/jp5072428
Dynamics Simulations with Spin-Flip Time-Dependent Density Functional Theory: Photoisomerization and Photocyclization
Mechanisms of *cis*-Stilbene in $\pi\pi^*$ States
Yu Harabuchi, Kristopher Keipert, Federico Zahariev, Tetsuya Taketsugu, and Mark S. Gordon*

11999  DOI: 10.1021/jp507282d
Ab Initio Study of Potential Ultrafast Internal Conversion Routes in Oxybenzone, Caffeic Acid, and Ferulic Acid: Implications
for Sunscreens
Tolga N. V. Karsili,* Barbara Marchetti, Michael N. R. Ashfold,* and Wolfgang Domcke

12011  DOI: 10.1021/jp507396e
A Multireference Configuration Interaction Study of the Photodynamics of Nitroethylene
Itamar Borges Jr.,* Adélia J. A. Aquino, and Hans Lischka*

12021  DOI: 10.1021/jp507520c
Role of Excitonic Coupling and Charge-Transfer States in the Absorption and CD Spectra of Adenine-Based
Oligonucleotides Investigated through QM/MM Simulations
Vincent A. Spata and Spiridoula Matsika*

12031  DOI: 10.1021/jp5076719
Role of Proton Hopping in Surface Charge Transport on Tin Dioxide As Revealed by the Thermal Dependence of
Conductance
Robert B. Wexler and Karl Sohlberg*

12041  DOI: 10.1021/jp507681g
Photochemical Deactivation Process of HCFC-133a ($C_2H_2F_3Cl$): A Nonadiabatic Dynamics Study
Gessenildo Pereira Rodrigues, Elizete Ventura,* Silmar Andrade do Monte, and Mario Barbatti*

12050 

DOI: 10.1021/jp507698m

Systematic Exploration of Minimum Energy Conical Intersection Structures near the Franck–Condon Region
Satoshi Maeda,* Yu Harabuchi, Tetsuya Taketsugu, and Keiji Morokuma

12059

DOI: 10.1021/jp507880q

Parallelization Strategy for Large-Scale Vibronic Coupling Calculations
Scott M. Rabidoux,* Victor Eijkhout, and John F. Stanton

12069

DOI: 10.1021/jp5090444

Short-Time Dynamics at a Conical Intersection in High-Harmonic Spectroscopy
Serguei Patchkovskii* and Michael S. Schuurman

12080 

DOI: 10.1021/jp509430p

Energy Disposal and Thermal Rate Constants for the OH + HBr and OH + DBr Reactions: Quasiclassical Trajectory Calculations on an Accurate Potential Energy Surface
Antonio G. S. de Oliveira-Filho,* Fernando R. Ornellas, and Joel M. Bowman

Articles

Kinetics and Dynamics

12089 

DOI: 10.1021/jp5072814

Theoretical Chemical Kinetic Study of the H-Atom Abstraction Reactions from Aldehydes and Acids by $\dot{\text{H}}$ Atoms and $\dot{\text{O}}\text{H}$, HO_2 , and CH_3 Radicals
Jorge Mendes, Chong-Wen Zhou,* and Henry J. Curran

12105

DOI: 10.1021/jp509856g

Conditions for Critical Effects in the Mass Action Kinetics Equations for Water Radiolysis
Richard S. Wittman,* Edgar C. Buck, Edward J. Mausolf, Bruce K. McNamara, Frances N. Smith, and Chuck Z. Soderquist

12111 

DOI: 10.1021/jp509990u

Formation of 6-Methyl-1,4-dihydronaphthalene in the Reaction of the *p*-Tolyl Radical with 1,3-Butadiene under Single-Collision Conditions
Dorian S. N. Parker, Beni B. Dangi, Ralf. I. Kaiser,* Adeel Jamal, Mikhail Ryazantsev, and Keiji Morokuma*

12120

DOI: 10.1021/jp511498r

Dynamics of the O + ClO Reaction: Reactive and Vibrational Relaxation Processes
O. B. M. Teixeira, P. J. S. B. Caridade,* V. C. Mota, J. M. Garcia de la Vega, and A. J. C. Varandas*

Spectroscopy, Photochemistry, and Excited States

12130  DOI: 10.1021/jp5075829

Methyl Internal Rotation in the Microwave Spectrum of Vinyl Acetate
Ha Vinh Lam Nguyen,* Atef Jabri, Vinh Van, and Wolfgang Stahl

12137  DOI: 10.1021/jp5081252

Structure–Property Relationships in an Iridium(III) Bis(Terpyridine) Complex with Extended Conjugated Side chains
Joachim Kübel, Andreas Winter, Ulrich S. Schubert, and Benjamin Dietzek*

12149  DOI: 10.1021/jp508340p

Solvent-Induced Frequency Shifts of 5-Hydroxymethylfurfural Deduced via Infrared Spectroscopy and *ab Initio* Calculations
Tyler R. Josephson, George Tsilomeleki, Christina Bagia, Vladimiro Nikolakis, Dionisios G. Vlachos, and Stavros Caratzoulas*

12161  DOI: 10.1021/jp510293k

Initial Excited-State Structural Dynamics of 6-Substituted Uracil Derivatives: Femtosecond Angle and Bond Lengthening Dynamics in Pyrimidine Nucleobase Photochemistry
Faranak Teimoory and Glen R. Loppnow*

12168  DOI: 10.1021/jp510712s

Conjugation in and Optical Properties of 1-*R*-1,2-Diphospholes and 1-*R*-Phospholes
Sergey A. Katsyuba,* Timur I. Burganov, Elena E. Zvereva, Almaz A. Zagidullin, Vasily A. Miluykov, Peter Lönnecke, Evamarie Hey-Hawkins, and Oleg G. Sinyashin

12178  DOI: 10.1021/jp511084w

Theoretical Assessment of the Selective Fluorescence Quenching of 1-Amino-8-naphthol-3,6-disulfonic Acid (H-Acid) Complexes with Zn^{2+} , Cd^{2+} , and Hg^{2+} : A DFT and TD-DFT Study
Pezhman Zarabadi-Poor and Joaquín Barroso-Flores*


12184  DOI: 10.1021/jp5111218

Photoreactivity of a Quantum Dot–Ruthenium Nitrosyl Conjugate
Lilian Pereira Franco, Simone Aparecida Cicillini, Juliana Cristina Biazotto, Marco A. Schiavon, Alexander Mikhailovsky, Peter Burks, John Garcia, Peter C. Ford,* and Roberto Santana da Silva*

Molecular Structure, Quantum Chemistry, and General Theory

12192  DOI: 10.1021/jp508979u

Role of Hydrogen Abstraction Acetylene Addition Mechanisms in the Formation of Chlorinated Naphthalenes. 1. A Quantum Chemical Investigation
Grant J. McIntosh* and Douglas K. Russell

-
- 12205  DOI: 10.1021/jp5089806
Role of Hydrogen Abstraction Acetylene Addition Mechanisms in the Formation of Chlorinated Naphthalenes. 2. Kinetic Modeling and the Detailed Mechanism of Ring Closure
Grant J. McIntosh* and Douglas K. Russell
-
- 12221  DOI: 10.1021/jp507924p
London Force Correction Disparity in the Modeling of Crystalline Asparagine and Glutamine
Thomas R. Juliano Jr. and Timothy M. Korter*
-
- 12229 DOI: 10.1021/jp5079949
Vibrations of Bionic Liquids by Ab Initio Molecular Dynamics and Vibrational Spectroscopy
Luana Tanzi, Paola Benassi, Michele Nardone, and Fabio Ramondo*
-
- 12241 DOI: 10.1021/jp508817v
Hydrogen-Bonding Interactions in Hard Segments of Shape Memory Polyurethane: Toluene Diisocyanates and 1,6-Hexamethylene Diisocyanate. A Theoretical and Comparative Study
Cuili Zhang, Jinlian Hu,* Xun Li, You Wu, and Jianping Han
-
- 12256  DOI: 10.1021/jp509933x
Carbon Dioxide Capture with the Ozone-like Polynitrogen Molecule Li_3N_3
Miquel Torrent-Sucarrat* and António J. C. Varandas*
-
- 12262 DOI: 10.1021/jp510180j
Extended Y-Rule Method for the Characterization of the Aromatic Sextets in Cata-Condensed Polycyclic Aromatic Hydrocarbons
Jorge O. Oña-Ruales* and Yosadara Ruiz-Morales
-
- 12274  DOI: 10.1021/jp510622u
Pair-Potential Approach to Accurate Dispersion Energies between Group 12 (Zn, Cd, Hg) Clusters
Richard Hatz, Vesa Hänninen, and Lauri Halonen*
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