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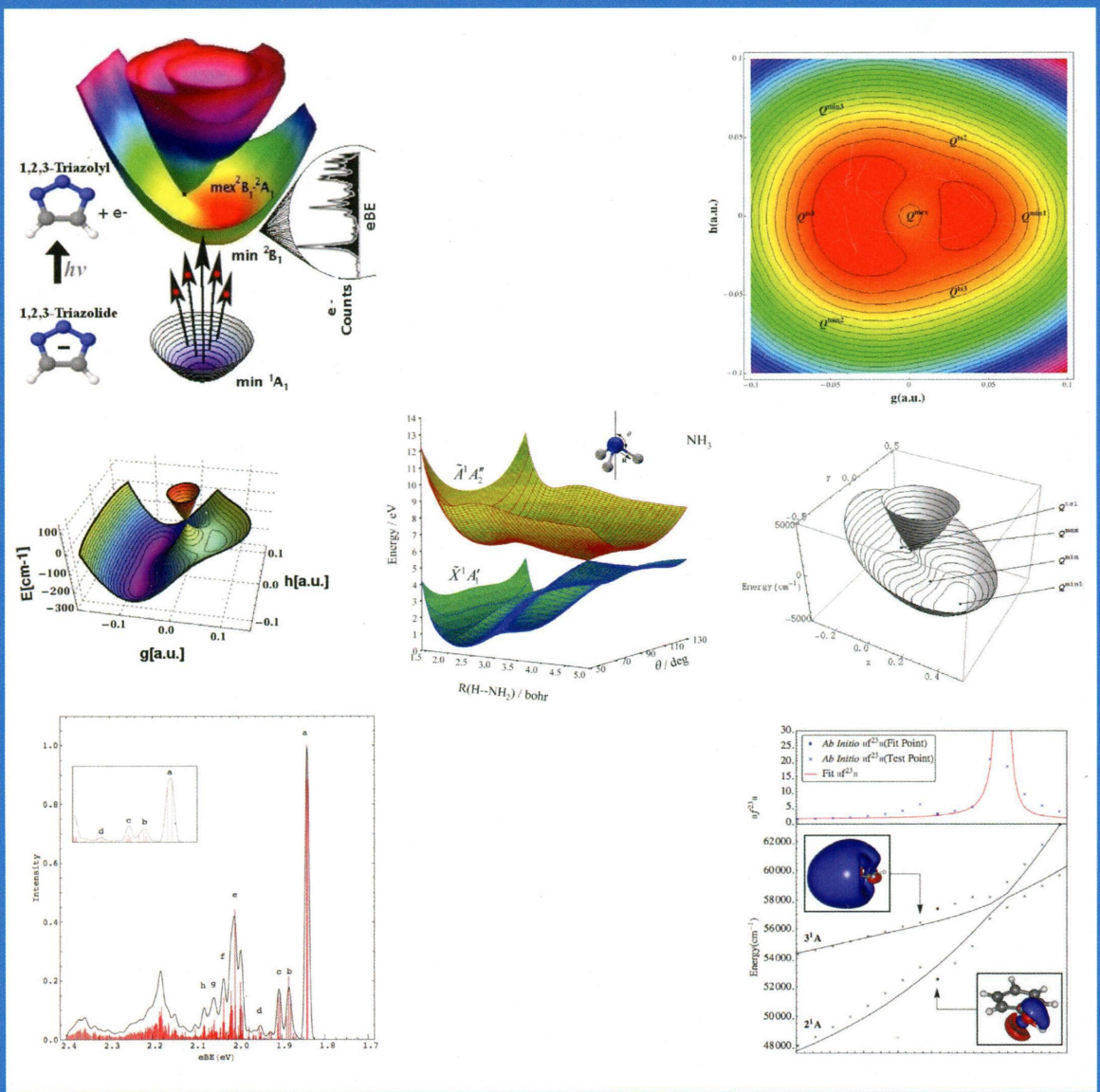

DAVID R. YARKONY FESTSCHRIFT

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

Articles

Articles

Kinetics and Dynamics

Spectroscopy, Photochemistry, and Excited States

Molecular Structure, Quantum Chemistry, and General Theory

Ⓢ Supporting Information available via online article