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### **Conical intersections: electronic structure, dynamics & by**

Section I of the book provides a comprehensive analysis of the electronic-structure aspects of conical intersections. Section II shows the importance of conical intersections in chemical reaction dynamics and gives an overview of the computational techniques employed to describe the dynamics at conical intersections.

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May 7, 2004 16:15 Conical Intersections: Electronic Structure, Dynamics and Spectroscopy index Index 831 crossing seam, 210 crude adiabatic basis, 66, 181

### **Conical Intersections: Electronic Structure, Dynamics**

May 22, 2004 9:5 Conical Intersections: Electronic Structure, Dynamics and Spectroscopy contents x Conical Intersections: Electronic Structure, Dynamics and Spectroscopy by electronic relaxation all the way to the ground state.

### **Conical Intersections: Electronic Structure, Dynamics**

Conical Intersections Electronic Structure, Dynamics and Spectroscopy Edited by: Wolfgang Domcke ( Technical University of Munich, Germany ), David R Yarkony ( John Hopkins University, USA ), Horst KÄppel ( University of Heidelberg, Germany )

### **BORN-OPPENHEIMER APPROXIMATION AND BEYOND | Conical**

The energy and structure of the quasi Jahn-Teller degeneracy which is between S3 and S2 are computed, as well as those of three conical intersections connecting S1 and S2.

### **Conical intersections and the electronic structure of the**

Jahn-Teller geometry is a conical intersection between the two components of a degenerate state. " Herzberg and Longuet-Higgins (1963) " a real-valued electronic wave function changes sign when the nuclear coordinates traverse a closed path encircling a conical intersection " geometric phase effect.

### **Conical Intersections, nonadiabatic couplings with**

Conical Intersections, ... model Hamiltonian for the electronic structure of a ... different decay pathways. We find that intersections between the S 1 and ...

### **Conical Intersections, Charge Localization and**

electronic effects, which help to explain and predict the structure and energetics of conical intersections. A three-step strategy for the conceptual search of conical intersections is outlined.

### **Geometrical and substituent effects in conical**

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Section 1 presents a brief overview of the history of conical intersections and their rise from an arcane theoretical concept to a major paradigm in nonadiabatic chemistry. In Section 2, the generic properties of conical intersections are discussed, as well as their characterization with modern electronic-structure methods.

**Role of Conical Intersections in Molecular Spectroscopy**

Domcke W, Yarkony DR, Köppel H (eds) (2004) Conical intersections: electronic structure, dynamics and spectroscopy. Advanced series in physical chemistry, vol 15.

**Comparison of algorithms for conical intersection**

photoisomerization – the conical intersection itself is a ten-dimensional manifold. The staggering dimensionality of intersection seams for more complicated systems (fig. 1) is quite difficult to grasp.

**Conical Intersections and Charge Localization in a Minimal**

conical intersections. To our knowledge, this is the first example whereby localized diabaticization techniques have been tested and have successfully recovered the topology of a conical intersection.

**Electronic Relaxation in Benzaldehyde Evaluated via TD-DFT**

Quantum Dynamics at Conical Intersections Edited by Stuart C. Althorpe School of Chemistry University of Nottingham ... the Conical Intersection Hyperline using Gradients, Second Derivatives, and Dynamics ... the fields of electronic structure theory, high-resolution spectroscopy, theoret- ...

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