

Accepted Manuscript

Theoretical Study on Electronic Excitation Spectra: A Matrix Form of Numerical Algorithm for Spectral Shift

Mei-Jun Ming, Long-Kun Xu, Fan Wang, Ting-Jun Bi, Xiang-Yuan Li

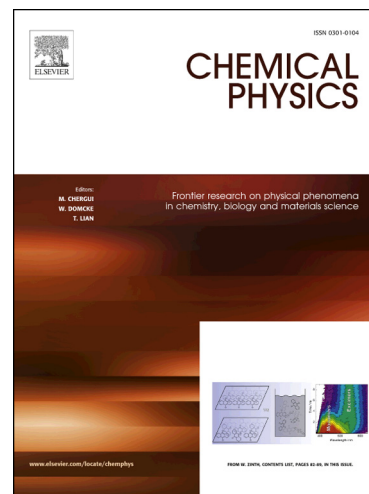
PII: S0301-0104(17)30139-8
DOI: <http://dx.doi.org/10.1016/j.chemphys.2017.05.016>
Reference: CHEMPH 9799

To appear in: *Chemical Physics*

Received Date: 27 February 2017
Accepted Date: 23 May 2017

Please cite this article as: M-J. Ming, L-K. Xu, F. Wang, T-J. Bi, X-Y. Li, Theoretical Study on Electronic Excitation Spectra: A Matrix Form of Numerical Algorithm for Spectral Shift, *Chemical Physics* (2017), doi: <http://dx.doi.org/10.1016/j.chemphys.2017.05.016>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Theoretical Study on Electronic Excitation Spectra: A Matrix Form of Numerical Algorithm for Spectral Shift

Mei-Jun Ming[†], Long-Kun Xu[§], Fan Wang[‡], Ting-Jun Bi[§], and Xiang-Yuan Li^{*,§}

[†]College of Chemistry, Sichuan University, Chengdu 610064, China

[§]College of Chemical Engineering, Sichuan University, Chengdu 610065, China

[‡]Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

*To whom correspondence should be addressed. E-mail: xyli@scu.edu.cn

ABSTRACT: In this work, a matrix form of numerical algorithm for spectral shift is presented based on the novel nonequilibrium solvation model that is established by introducing the constrained equilibrium manipulation. This form is convenient for the development of codes for numerical solution. By means of the integral equation formulation polarizable continuum model (IEF-PCM), a subroutine has been implemented to compute spectral shift numerically. Here, the spectral shifts of absorption spectra for several popular chromophores, *N,N*-diethyl-*p*-nitroaniline (DEPNA), methylenecyclopropene (MCP), acrolein (ACL) and *p*-nitroaniline (PNA) were investigated in different solvents with various polarities. The computed spectral shifts can explain the available experimental findings reasonably. Discussions have been made on the contributions of solute geometry distortion, electrostatic polarization and other non-electrostatic interactions to spectral shift.

Highlights

► A novel expression of nonequilibrium solvation energy is presented by introducing the constrained equilibrium approach, which is different from the traditional ones. ► A matrix form of numerical formula for spectral shift is presented and the computational codes have been implemented by combining with PCM. ► Solvent effects on electronic excitation spectra of several chromophores were investigated and discussed.

Keywords: Nonequilibrium solvation, Spectral shift, Constrained equilibrium, Vertical excitation energy, Numerical algorithm

1. Introduction

Download English Version:

<https://daneshyari.com/en/article/5372590>

Download Persian Version:

<https://daneshyari.com/article/5372590>

[Daneshyari.com](https://daneshyari.com)