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2nd EAI International Conference on Future Access Enablers of Ubiquitous and Intelligent Infrastructures

OCTOBER 24-25, 2016 | BELGRADE, SERBIA

FABULOUS 2016 PROGRAM

Monday, 24 Oct 2016

09:30-10:00 Conference opening  Prof. Nenad Filipovic - Faculty of Engineering, University of Kragujevac - FABULOUS 2016 General Chair

10:00-10:45 Keynote speech  Prof. Liljana Gavrilovska, Faculty of Electrical Engineering and Information Technologies, Sts. Cyril and Methodius University in Skopje, Macedonia
SG: the Dawn of the new Era

10:45-11:30 Keynote speech  Dr. Prof. Onur Mutlu, ETH Zurich, Switzerland
Rethinking Memory System Design for Data-Intensive Computing

11:30-11:45 Sponsor presentation  Dusan Vukasinovic, Andjelko Cajkovic, National Instruments

11:45-12:15 Coffee break

12:15-13:45 FAN 2016  Chair: Prof. Onur Mutlu, ETH Zurich, Switzerland

- Milos Radovic, Milos Jordanski and Nenad Filipovic, "T-Relief: Feature Selection for Temporal High-Dimensional Gene Expression Data"
- Bojan Markinkovic, Paolo Glavain and Zoran Ognjanovic, "Correctness of the Chord Protocol Using the Frame of the Logic of Time and Knowledge"
- Fadi AlTurjuman, "Identification Framework for Smart Environments in the Era of Cloud-IoT"
- Radu Alexandru Badea, Octaviana Dalcu and Robert Dobro, "A Multi-Level Protocol Stack for Flexible and Secure Client-App to Cloud Communication"
- Tijana Sustercic, Aleksandra Vukovic, Nenad Filipovic and Aleksandar Peulic, "FPGA Implementation of Face Recognition Algorithm"
- Tijana Djekic and Nenad Filipovic, "Parallelization of the numerical simulation of motion of deformable objects within fluid domain on a GPU device"
- Alexandru Stanca, Stefan Arseni, Alexandru Vulpe, Octavian Fratu and Simona Halunga, "Intrusion Prevention System Evaluation for SDN-enabled IoT Networks"
- Ivan Petrov, Prof. Toni Janevski "5G-TCP: Enhanced transport protocol for Future Mobile Networks"
- Ioana Marcu, Carmen Voicu, Simona Halunga and Radu Preda, "LDPC encoding performances for fading suppression in MIMO-CDMA wireless networks"

13:45-14:45 Lunch

14:45-15:30 Keynote speech  Prof. Dimitrios I. Fotiadis, University of Ioannina, Greece
Fighting for a healthcare environment based on mobile solutions
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<td>15:30-16:00</td>
<td>Coffee break</td>
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<td>16:00-18:20</td>
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**Chair:**

Prof. Dimitrios I. Fotiadis, University of Ioannina, Greece

- Nikola Mljakovic, Radivoje Radakovic, Aleksandar Peulic, Neda Vidanovic, Djordje Dimitrijevic and Nenad Filipovic, "Assessment of mechanical stiffness of jumping using force plate"
- Bojana Andjelkovic Cirkovic, Aleksandar Cvetkovic, Danijela Cvetkovic, Srdjan Ninkovic and Nenad Filipovic, "Prediction of the Five Years Survival Rate for Breast Cancer Patients within the Ensemble Feature Ranking Framework"
- Lejla Gurbeta, Almir Badoravc, Zijad Dzemic, Elvira Ruiz Jimenez and Alma Jakupovic, "Testing of Therapeutic Ultrasound Equipment in Healthcare Institutions in Bosnia and Herzegovina"
- Krasimir Tonchev, Georgi Tsenov, Valeri Miadenov, Agata Manolova and Vladimir Pouklov, "Personalized and intelligent sleep lifestyle reasoner with web application for improving quality of sleep part of AAL architecture"
- Aleksandra Vukovic, Tijana Sustercic, Vesna Rankovic, Aleksandar Peulic and Nenad Filipovic, "Comparison of Different Neural Network Training Algorithms with Application to Face Recognition Problem"
- Marko Zivanovic, Danijela Cvetkovic and Nenad Filipovic, "uSense Cancer Procedure for Detection of microRNAs as Cancer Biomarkers - From Science to Patients"
- Strahinja Starcevic, Smiljana Djorovic and Nenad Filipovic, "Fractional Flow Reserve: Comparison between Invasive and Non-invasive Methods for Calculation of FFR"
- Igor Savelic, Velibor Isailovic, Lazar Yelicki, Dalibor Nikolic and Nenad Filipovic, "Numerical modeling and simulations of type B aortic dissection"
- Smiljana Djorovic, Igor Koncar, Lazar Davidovic, Strahinja Starcevic and Nenad Filipovic, "Computational Analysis of Blood Flow Characteristics in an Aortic System with Abdominal and Left Common Iliac Aneurysm Pre- and Post-Stent Grafting"
- Arso M. Vukcevic, Gordana Jovic, Nebojsa Jovicic and Nenad Filipovic, "Estimating Cortical Bone Fracture Resistance by using Artificial Neural Networks and Linear Regression"
- Velibor Isailovic, Milica Nikolic, Thanas Bitas, Antonis Sakellarios, Nikolas Tachos, Miljan Milosevic and Nenad Filipovic, "Numerical simulation of human hearing system"
- Miljan Milosevic, Vladimir Simic and Milos Kojic, "Numerical modeling of drug delivery in organs: from CT scans to FE model"
- Dalibor Nikolic, Igor Savelic, Milos Radovic and Nenad Filipovic, "Shear stress in the arteries with myocardial bridge "solved" by neural networks"

**20:00:** Gala dinner

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**Tuesday, 25 Oct 2016**

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<tr>
<td>10:00-10:45</td>
<td>Keynote speech</td>
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Dr. Emi Jovanov, University of Alabama in Huntsville,
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<th>Time</th>
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| 10:45-12:15  | EnFuSi 2016                                | **Chair:** Dr. Emil Jovanov, University of Alabama in Huntsville, USA  
**“Smart Stuff and Wearable Monitoring”**  
- George Suciu, Iulia Rotaru, Ana-Maria Coman and Octavian Fratu, “Tele-Monitoring the Battery of an Electric Vehicle”  
- Radu Mihaea Udrea, Claudia Cristina Oprea and Cristian Stanciu, “Multi-microphone Noise Reduction System Integrating Nonlinear Multi-Band Spectral Subtraction”  
- George Suciu, Octavian Fratu, Victor Suciu and Iulian Grigore, “Monitoring the Black Sea Region using Satellite Earth Observation and Ground Telemetry”  
- Elena-Madalina Oprea, Alexandru Razvan Vulpe, Ion Marghescu and Octavian Fratu, “High Capacity Ethernet Radio Relay Networks in Mobile Communications”  
- Konstantin Chornu, Vladimir Atanasovski, Uliana Gavrilevskina and Michele Magno, “Practical Implementation Aspects of the Data Timed Sending (DTS) Protocol Using Wake-up Radio (WuR)”  
| 12:15-12:45  | Coffee break                               |                                                                                                   |
| 12:45-14:15  | Keynote speech                             | Prof. Veljko Milutinovic, School of Electrical Engineering, University of Belgrade, Serbia  
**“DataFlow SuperComputing for DataAnalytics”**  
| 14:15-15:15  | Lunch                                      |                                                                                                   |
| 15:15-15:35  | DaMBIC 2016                                | **Chair:** Prof. Veljko Milutinovic, University of Belgrade, Serbia  
**“Tractable Policy Management Framework for Cognitive IoT”**  
**“Vestislava Stoykova, ‘Extracting Academic Subject Semantic Relations Using Collocations’”**  
| 15:35-16:05  | Computational Chemistry                    | **Chair:** Prof. Zeljko Cupic, Institute of Chemistry, Technology and Metallurgy, Belgrade  
**“Experimental and theorectical study of the UV-Vis spectrum of a new coumarine-derived ligand”**  
**“Jelena Djorovic, Zoran Markovic, Svetlana Jeremic and Dejan Milenkovic, ‘Investigation of the antioxidative and radical scavenging activities of 2,4-, 2,5-, 3,5-dihydroxybenzoic acids’”**  
**“Svetlana Jeremic, Dejan Milenkovic, Milos Filipovic, Slavko Radenkovic, Marija Ante, Zoran Markovic, ‘Importance of Some Conceptual DFT Reactivity Indices in QSAR Modelling of the Antioxidative Capacity of Simply Phenolic Antioxidants’”**  
|
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31 July 2016

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  Workshop Chair: Prof. Emil Jovanov, USA

• Workshop #3: Data Mining, Big Data and Cloud Computing
  Workshop Chair: Cemir Mutlu, Carnegie Mellon University

• Workshop #4: eHealth and Biomedical engineering
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<td>University of Novi Sad</td>
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Experimental and theoretical study of the UV-Vis spectrum of a new coumarine-derived ligand

Dejan Milenković*, Srečko Trifunović, Edina Avdović, Nenad Vuković, Milena Vukić, Jasmina Dimitrić-Marković, and Zoran Marković

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3Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16,11000 Belgrade, Republic of Serbia
4Department of Chemical-Technological Sciences, State University of Novi Pazar, Vuka Karadžića bb, 36300 Novi Pazar, Serbia

Abstract. The UV-Vis properties of new coumarine-derived ligand (3-(1-(3-hydroxypropylamino)propyldene)-chroman-2,4-dione) were investigated. The time-dependent density functional theory (TDDFT) approach in combination with the B3LYP functional was used for simulation of UV-Vis spectra of examined compound. The agreement between the observed wavelengths and intensities in the UV spectrum of ligand 1 and those predicted with B3LYP functional, is satisfactory.

Keywords: UV-Vis spectra, TDDFT, B3LYP, coumarine-derived ligand (ligand 1), oscillator strengths

1 Introduction

Coumarins (2H-1-benzopyran-2-one) consist of a large class of phenolic substances found in plants and are made of fused benzene and α-pyrene rings [1]. Coumarine and its derivatives are natural compounds with high and significant bilogical activities like spasmolitic, antiarrhythmic, cardiotonic and photodynamic properties [2]. Also, coumarine and its derivatives were tested against several tumor cell lines [3]. These compounds can be found in different food sources such as fruits, herbs and vegetables [4]. Coumarin and its derivatives have important role in the fields of biology, medicine, industry, botany and chemistry. Some metal complexes with coumarine derivatives showed significant anticoagulant [5] and antitumor activity [2,6].

* Dejan Milenković, Bioengineering Research and Development Center, Prvoslava Stojanovića 6, 34000 Kragujevac, Serbia (deki82@kg.ac.rs)
2 Methodology section

The equilibrium geometry of coumarine-derived ligand (1) was optimized by density functional theory (DFT) using B3LYP exchange correlation functional first proposed by Becke [7], in combination with the 6–311+G(d,p) basis set. The optimization was carried out using Gaussian 09 package [8]. The structure was optimized at 298 K without any geometrical restrictions. The nature of the stationary points was determined by performing frequency analysis: equilibrium geometries have no imaginary vibrations. The effect of methanol as solvent was taken into account in geometry optimization and energy calculation by using the SMD model [9].

To simulate the UV spectrum of investigated compound TDDFT (Time Dependent Density Functional Theory) approach [10] was employed for predicting the electronic transitions. TD calculation was performed in methanol. All transitions were considered. All parameters important for the simulation of UV-VIS spectra such as excited state energies, oscillator strengths (f), and a list of the transitions that gave rise to each excited state were calculated. Natural Bond orbital (NBO) analysis [11] was performed for the explanation of the interactions inside of molecule and visualization of orbitals involved in electronic transitions. The B3LYP ground state geometry was used to perform the NBO.

3 Results and discussion

3.1 Structural analysis

The structure of most stable conformation of ligand 1 defined by using B3LYP local density functional method in conjunction with 6–311+G(d,p) basis set, in methanol as solvent. From the optimized molecular structure of the ligand 1 (Fig. 1), it is found that torsion angle, τ, defined by the C4–C3–C1′–N1 atoms is 172°, which indicated nonplanarity of molecule. The investigated molecule has one internal hydrogen bond (IHB) which additionally stabilize corresponding compound. For this IHB the NBO analysis revealed that electron density is donated from the p and sp² orbitals of the oxygen atoms into the proximate σ* antibonding H–N1 bond. These donor-acceptor interactions are responsible for hydrogen bond formation.
3.2 UV spectrum

The experimental and computed UV spectra are presented in Fig. 2, whereas calculated electronic transitions, absorption wavelengths, and oscillator strength, as well as experimental absorption wavelengths are presented in Table 1.

Table 1. UV spectral data for compound 1.

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<th>Expt</th>
<th>B3LYP/6-311+G(d,p)</th>
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<tbody>
<tr>
<td>$\lambda_{\text{max}}$ (nm)</td>
<td>$\lambda_{\text{max}}$</td>
<td>$f$</td>
</tr>
<tr>
<td>319</td>
<td>294</td>
<td>0.52</td>
</tr>
<tr>
<td>243</td>
<td>248</td>
<td>0.18</td>
</tr>
<tr>
<td>234</td>
<td>238</td>
<td>0.28</td>
</tr>
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The experimental spectrum of 1 in of methanol shows two wide peaks at 319 and 243 nm. The theoretical investigation of electronic transition was also performed in methanol. The UV spectrum of the compound 1 was simulated using the TDDFT approach. In Table 1 are given data for the UV spectrum. The two absorption peaks are prominent, i.e., at 294 nm which is absorption maximum and the second peak has been observed at 248 nm which are in good agreement with the experimental evidences (Table 1, Fig. 2). As mentioned above, electronic transitions have been investigated. The first transition state at 294 nm dominated with maximum absorption which is caused by HOMO →LUMO with 66% contribution. The second transition state caused by HOMO → LUMO+1 at 248 nm with 48% contribution. The third state has 58% contribution from HOMO-1 → LUMO+1. The orbitals corresponding for these electronic transitions were presented in Fig. 3.
Figure 2. Experimental (blue line) and simulated (red line) UV spectrum of ligand 1 in methanol. The calculation of the spectrum was carried out at the B3LYP-D3/6-311+G(d,p) level of theory in combination with the SMD solvation model.

Figure 3. The occupied and virtual orbitals responsible for the UV spectrum of ligand 1.
The shapes of the corresponding orbitals confirm that these transitions were associated with significant charge transfer between the coumarine moiety and side alkyl chain.

4 Conclusion

All results were obtained using the B3LYP/6-311+G(d,p) level of theory. On the basis of conformational analysis, it was found that 1 is the most stable structure. Re-optimized structure of 1 in methanol was used to simulate the UV–vis spectra. Both methods, experimental and theoretical showed as two major peaks. The results showed that there is good agreement between experimental and calculated values for \( \lambda_{\text{max}} \). On the basis of new facts, it is clear that this functional (B3LYP) can be used successfully in the study of this class of compounds. According to the analysis of frontier orbitals it was found that for these transitions was responsible charge transfer between the coumarine moiety and side alkyl chain.

Acknowledgments. This work was supported by the Ministry of Science of the Republic of Serbia (Projects Nos. 172015, 174028 and 172016).

References

