Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Abstract. In this present work, we calculated two frontier orbital energies - singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) - of dehydrogenated tetrahydrocurumin (THC) using density-functional theory (DFT) in gas phase. We used the energy difference of SOMO and LUMO to assess the stability of dehydrogenated THC after performing a hydrogen atom transfer toward reactive oxygen species (ROS). We began by optimizing dehydrogenated THC at six hydrogen abstraction sites. Two hydrogen abstraction sites are at O-H groups and four hydrogen abstraction sites are at C-H groups. Then, we compared the value of SOMO and LUMO energy difference in each site. Our calculations showed that dehydrogenated THC at O-H groups are more stable than dehydrogenated THC at C-H groups.

1. Introduction

Hydrophilic reactive oxygen species (ROS) is able to penetrate into phospholipid bilayer membrane and oxidizes the membrane [1,2] by abstracting a hydrogen atom. This abstraction process marks the beginning of oxidation chain called lipid peroxidation. Since cell membrane is the outermost part of a cell that protects its organelles, oxidation by ROS may lead to pores formation on the membrane [3] and eventually to a cell degradation.

In order to delay or prevent this oxidation process, one can introduce a molecule that performs antioxidant activity which is the ability to transfer hydrogen atom toward ROS to break an oxidation chain[4,5]. An electron paramagnetic resonance study has shown that tetrahydrocurcumin (THC) molecule possesses slightly better antioxidant activity than its former, curcumin molecule [6]. THC also performs an inhibitory effect on membrane lipid peroxidation, experimentally [7].

Since THC can possibly perform its antioxidant activity by transfering a hydrogen atom, the aim of our research is to calculate the energy difference between frontier orbitals of dehydrogenated THC (dehydrogenated THC is THC that has transferred its hydrogen atom) in gas phase, theoretically. We use density functional theory (DFT) to evaluate two frontier orbital energies of dehydrogenated THC, which are singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) energies. The energy difference between SOMO and LUMO will help us to assess the most possible site in THC that is responsible for antioxidant activity of the molecule, which is the dehydrogenated THC with the highest energy difference in its frontier orbitals.

2. Computational details

THC performed its antioxidant activity by transferring one of its hydrogen atom. In this research, we chose six representative X-H sites that were capable of transferring a hydrogen atom (see figure 1). To calculate the energy difference between frontier orbitals of dehydrogenated THC, we conducted our research in the following steps. First step, we built a dehydrogenated THC by abstracting a hydrogen atom from each X-H sites. Each THC with one less hydrogen atom was called dehydrogenated THC 1, dehydrogenated THC 2, etc. Dehydrogenated THC 2 and dehydrogenated THC 5 were produced as a result of a hydrogen atom abstraction from an O-H groups. While other dehydrogenated THCs were produced as a result of a hydrogen atom abstraction from a C-H groups. Although experimental result has suggested that O-H groups played an important role in hydrogen atom transfer [8], we propose to consider the presence of C-H bonds as well in this research. Our molecule of interest has a symmetrical shape. This means if we draw a line at the center of the molecule, the line will divide the molecule into two equal parts. Thus, among the six representative sites chosen, site 1 was in the same position as site 6, site 2 was in the same position as site 5 and site 3 was in the same position as site 4.

Second step, after building six dehydrogenated THCs, we performed full geometry optimisation using UM05-2X functional and 6-31++G(d,p) basis set. M05-2X functional was chosen because it has been recommended for thermochemistry calculations by its developer [9]. We used an unrestricted calculation (symbolled by letter U) since dehydrogenated THC has lost one electron during the hydrogen abstraction so we treated it as an open shell calculation. The geometry optimisation was calculated using DFT applied in Gaussian 09 suite program [10] in gas phase at 298.15 K. At this step, our calculation produced the frontier orbital energies.

Our last step is to find the energy difference between two frontier orbital energies, which are SOMO and LUMO energies at each dehydrogenated THC.

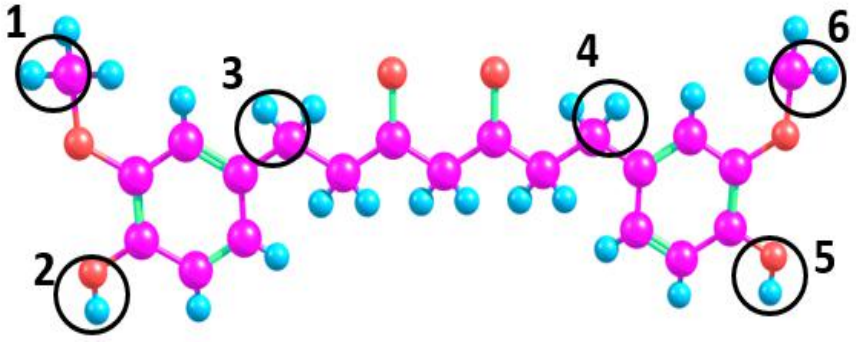

Figure 1. Six representative X-H sites (Blue, pink and red represent H, C and O atoms sequentially). Site 1, 3, 4 and 6 are C-H groups while site 2 and 5 are O-H groups.

3. Results and discussion

Figure 2 showed how model of dehydrogenated THC 2 was built. We built other dehydrogenated THCs with the same procedure. Since dehydrogenated THC 2 has lost one of its electron and proton (recall that we have abstracted a hydrogen atom from THC), we performed geometry optimisation by setting the spin multiplicity into 2 to make sure that the dehydrogenated THC 2 as well as other dehydrogenated THCs were at doublet state.

Figure 3 illustrated the SOMO and LUMO profiles of dehydrogenated THC 2. The SOMO profile was located at the hydrogen transferring sites. The profile informed us the location with the possibility of transferring electrons. After abstracting one hydrogen atom which contains of one proton and one electron, THC molecule was left with only one electron in its last occupied orbital. Thus this orbital was called SOMO. Differ from SOMO profile, LUMO profile was located at the center of the molecule. This profile informed us about the area possible of receiving electrons. Generally, SOMO profiles of all six dehydrogenated THCs were located at transferring sites while their LUMO profiles were located at the center of the molecule.

Our DFT calculation produced many orbital energies of dehydrogenated THCs. We chose two frontier orbitals, SOMO and LUMO, to assess the stability of dehydrogenated THCs[11]. Low energy difference between SOMO and LUMO meant an electron can easily be excited from its ground state, thus a molecule was less stable. While high energy difference between SOMO and LUMO meant an electron can be more stable in its ground state, thus a molecule was more stable.

We calculated energy difference between SOMO and LUMO, which we called it as relative SOMO-LUMO energies, of all six dehydrogenated THCs and tabulated the value in the graph at figure 4. The value of relative SOMO-LUMO energies at dehydrogenated THC 1 (site 1) and dehydrogenated THC 6 (site 6) was almost similar. Their difference was less than 0.2 eV. However, the value are very similar at dehydrogenated THC 2 (site 2) and dehydrogenated THC 5 (site 5), as well as at dehydrogenated THC 3 (site 3) and dehydrogenated THC 6 (site 6). The value of relative SOMO-LUMO energies from the highest to the lowest is dehydrogenated THC 2 = dehydrogenated THC 5 > dehydrogenated THC 1 > dehydrogenated THC 6 > dehydrogenated THC 3 = dehydrogenated THC 4. These results implied that dehydrogenated THC 2 was as stable as dehydrogenated THC 5. Both dehydrogenated THCs were the most stable among all six dehydrogenated THCs. Dehydrogenated THC 1 and 6 were less stable while dehydrogenated THC 3 and 4 had the lowest stability. Based on THC's similarity, site at the same position, possessed similar characters.

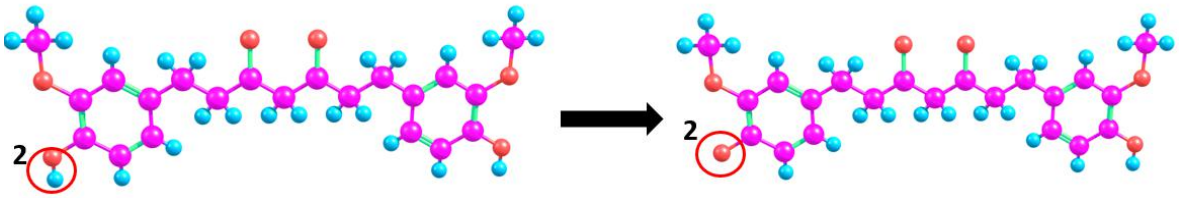

Figure 2. Model of dehydrogenated THC 2

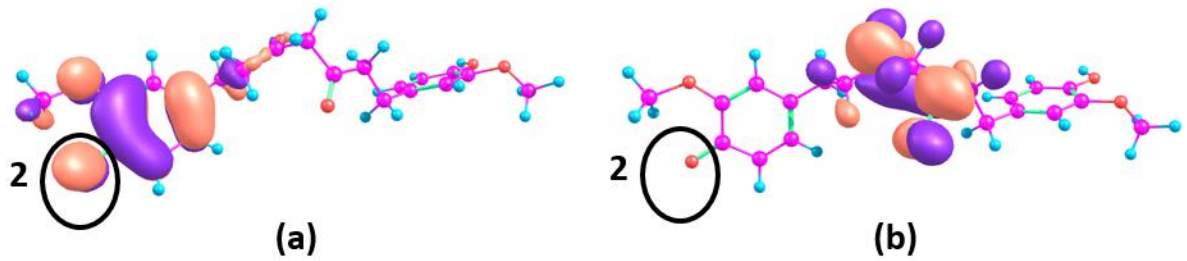

Figure 3. (a) SOMO and (b) LUMO profiles of dehydrogenated THC 2.

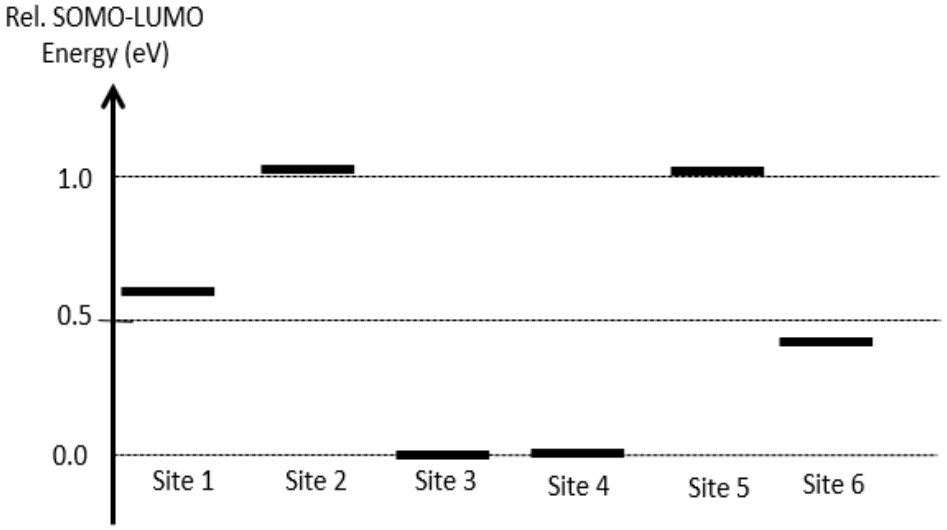

Figure 4. Relative energy diagram of dehydrogenated THC. X axes of the graph is the type of dehydrogenated THC while Y axes of the graph shows the energy difference between SOMO and LUMO.

Finally, in order to assess the most possible site in THC that was responsible for antioxidant activity of the molecule, we concluded the following information. To perform its antioxidant activity, THC should be able to transfer one of its hydrogen atom toward ROS. If the hydrogen atom transferred was originally from an O-H groups, after the transfer process dehydrogenated THC formed would be the most stable. This occured in the case of dehydrogenated THC 2 and 5. However, if the hydrogen atom transferred was originally from a C-H groups, after the transfer process dehydrogenated THC formed would be less stable. This occured in the case of dehydrogenated THC 1, 3, 4 and 6. After performing its antioxidant activity, THC should be able to maintain its stability. Thus the most possible site that is responsible for this activity is O-H groups of THC molecule.

4. Conclusion

We have performed DFT calculation to calculate frontier orbitals of six dehydrogenated THCs. We investigated two frontier orbitals of dehydrogenated THCs, SOMO and LUMO, to assess the stability of the molecules. We suggested that in performing its antioxidant activity, hydrogen atom transfer should occur from O-H groups of THC, since the dehydrogenated THC formed was the most stable. Thus, O-H groups were responsible for the antioxidant activity of THC. This conclusion was supported by our results in two previous researches [12-13].

Acknowledgement

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Table of contents

Volume 1204

April 2019

Previous issue Next issue

7th Asian Physics Symposium 29–31 August 2017, Bandung, Indonesia

Accepted papers received: 05 March 2019
Published online: 07 May 2019

View all abstracts

Preface

Papers

OPEN ACCESS 012025

Effect of Higher Order Thinking Virtual Laboratory (HOTVL) in Electric Circuit on Students' Creative Thinking Skills

S Sapriadil, A Setiawan, A Suhandi, A Malik, D Safitri, S A S Lisdiani and N Hermita

+ View abstract View article PDF

OPEN ACCESS 012026

Reducing Eleventh-Grade Students' Misconceptions on Gravity Concept using PDEODE ∗E-Based Conceptual Change Model

A Zulfikar, D Saepuzaman, H Novia, A H Setyadin, D S Jubaedah, F N Sholihat, M H Muhaemin, N F Afif, N J Fratiwi, S S Bhakti, S A Amalia, S R Hidayat, Z Nursani, N Hermita, B Costu and A Samsudin

+ View abstract View article PDF

OPEN ACCESS 012027

Optimizing Students' Conceptual Understanding on Electricity and Magnetism through Cognitive Conflict-Based Multimode Teaching (CC-BMT)

A Samsudin, A Suhandi, D Rusdiana, I Kaniawati, N J Fratiwi, A Zulfikar, M H Muhaemin, N Hermita, Mansur, F C Wibowo, Supriyatman, A Malik and B Costu

+ View abstract View article PDF

OPEN ACCESS 012028

Enthalpy of Formation of Na_xCoO_2 and $(Na, Mg)_xCoO_2$ Systems: A First Principle Calculation Study

Ivan Kurniawan and Bambang Prijamboedi

+ View abstract View article PDF

OPEN ACCESS 012029

Phenomenology of Minimal Composite Double Higgs Model

Bayu Adi Nugraha Putra and Jusak Sali Kosasih

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OPEN ACCESS 012030

Characterization of Calcium Powders from Merauke Mangrove Crab Shells

K Dahlan, E Haryati, O Togibasa and K Dahlan

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OPEN ACCESS 012031

Protein and Minerals Analyses of Mangrove Crab Shells (*Scylla serrata*) from Merauke as a Foundation on Bio-ceramic Components

E Haryati, K Dahlan, O Togibasa and K Dahlan

+ View abstract View article PDF

OPEN ACCESS 012032

Characterization of Tartaric-Sulphuric Acid Anodized 2024-T3 Aluminium Alloys with Anodizing Potential Variation

M H Setianto and Akhmad A. Korda

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OPEN ACCESS 012041

Preliminary Study on Electrical Properties of Hydrocarbon-Contaminated Soils at an Artisanal Oil Field in Central Java, Indonesia

E. Agustine, I D Dimawani, D. Fitriani, T D Pambudi, W. Srigutomo, S J Fajar and Trimadona

+ View abstract View article PDF

OPEN ACCESS 012042

Excavating the Quality of Vocational Students' Mental Models and Prediction on Heat Conduction

I M Sari, D Fauzi, A Malik, D Saepuzaman, T R Ramalis and D Rusdiana

+ View abstract View article PDF

OPEN ACCESS 012043

3-D Modeling of Time Domain Electromagnetic (TDEM) Method to Analyze the Layered Earth Structure in the Geothermal Systems

Cahyo Aji Hapsoro, Wahyu Srigutomo and Acep Purqon

+ View abstract View article PDF

OPEN ACCESS 012044

The Field Localization of Yukawa Interaction in a Modified Randall-Sundrum Model

Dewi Wulandari, Triyanta, Jusak S. Kosasih and Douglas Singleton

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OPEN ACCESS 012045

Enhancing Junior High School Students Conceptual Understanding Using the POE-based Demonstration Technique on Electrostatics

M G Purwanto, S R Hidayat, N J Fratiwi, A Zulfikar, M H Muhaimin, S S Bhakti, F N Sholihat, A H Setyadin, D S Jubaedah, S A Amalia, N F Afif, A Sutiadi, N Hermita and A Samsudin

+ View abstract View article PDF

OPEN ACCESS 012046

Promoting Oral-Communication Skill to the students of Seventh Grade on Earth Science Content Using Multimedia Based Integrated Instruction (MBI_2)

A H Setyadin, S R Hidayat, S S Bhakti, A Zulfikar, N J Fratiwi, M H Muhaimin, S A Amalia, D S Jubaedah, F N Sholihat, M G Purwanto, N F Afif, D T Chandra, P Siahaan, E Suhendi, I Kaniawati and A Samsudin

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OPEN ACCESS 012047

Hexagonal close-packed stability in two-dimensional selfgravitation granular particles system

P M Widartiningsih, S N Khotimah, B Dermawan and S Viridi

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Constructing Essay Questions To Assess Scientific Creative And Critical Thinking Simultaneously Related To Collision Problem Based On Students Responses

Iyon Suyana, Sarah Nadaipah, Parlindungan Sinaga and Selly Feranie

+ View abstract View article PDF

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Analyzing Students Responses To Construct Open Ended Question To Assess Scientific Creative And Critical Thinking (SCCT-Test) Related To Hydrostatic Pressure

H Rusnayati, N Oktavianti, H Novia, D Saepuzaman and S Feranie

+ View abstract View article PDF

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Geomagnetic Map of Field Camp Geophysics in Karangsambung using Data Acquisition 2005-2017

Eko Januari Wahyudi and Dedi Sukmayadi

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OPEN ACCESS 012051

Antibacterial Investigation Activity of Titania Anatase technical grade on polypropylene sheet

D O Margaretta, K W Permadi, D Y Rahman, F D Utami, S Viridi and M Abdullah

+ View abstract View article PDF

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Calculation of the binding energy of the lithium nucleus with the yukawa potential and the hellmann potential using WKB approximation

Ahmad Suaif, Dina Rahmawati and Zaki Su'ud

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The Effect of Hydrophilic Coating on Concrete Pile Surface in Pile Driving: Field Test

Nadya Amalia, Elfi Yuliza, Mamat Rokhmat, Edy Wibowo, Sparisoma Viridi and Mikrajuddin Abdullah

+ View abstract View article PDF

OPEN ACCESS 012054

Engaging Students in STEM Based Learning Through Media and Technology

I R Suwarma, I Kaniawati and D S Kaniawati

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Thermophysical parameters of organic PCM coconut oil from the T-history method and its variation with the chemical dopant

Alfriska O Silalahi, I M Sutjahja, D Kurnia and S Wonorahardjo

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The role of particle dopant to the thermal conductivities of PCM coconut oil by means of the T-history method

I M Sutjahja, Alfriska O Silalahi, D Kurnia and S Wonorahardjo

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The enthalpy-temperature curve of new PCM $Ca(NO_3)_2.4H_2O$ and $Co(NO_3)_2.6H_2O$ for low-temperature latent TES

Alfriska O Silalahi, I M Sutjahja, D Kurnia and S Wonorahardjo

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Identifying pre-service physics teacher mental model on electric conceptions

Supriyatman, Andi Suhandi, Dadi Rusdiana, Achmad Samsudin and Firmanul C. Wibowo

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Thermal Effect on Electromagnetic Suspension for Air Gap Performance in Magnetic Levitation System

Deny Viviantoro, Aliq Zuhdi, Agus Purbhadi and Mujamilah

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OPEN ACCESS 012060

The development of higher order thinking laboratory (hotlab) model related to heat transfer topic

A Malik, A Setiawan, A Suhandi, A Permanasari, A Samsudin, Y Dirgantara, H Y Suhendi, I M Sari and N Hermita

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OPEN ACCESS 012061

Radiation shielding design of neutron source from Kartini reactor's beam-port for SAMOP test facility

Tegas Sutondo and Syarip

+ View abstract View article PDF

Syuhada Syuhada, Nanang Tyasbudi Puspito, Titi Anggono, Nugroho Dwi Hananto, Hendra Grandis and Tedi Yudistira

+ View abstract View article PDF

OPEN ACCESS 012070

Geochemical Characteristics of Volcanic Rocks from Mt. Masurai's Caldera, Jambi, Indonesia

Asep Rohiman, Dipowiguno Prijanto, Arief Prabowo, Antonius Ratdomopurbo, Ruly Setiawan, Mutiara Effendi and Eko Wahyudi

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Myocardial infarction detection system from PTB diagnostic ECG database using Fuzzy inference system for S-T waves

A N Ardan, Miftahul Ma'arif, Z H Aisyah, M Olivia and S M Titin

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OPEN ACCESS 012072

Optimalization of ultrasonic tomography method using robotic instrument

Tedy Setiawan, Fatkhan, Fernando Lawrens and Albertus Ariel Rahadi

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Diagnosis of Student's Misconception on Momentum and Impulse Trough Inquiry Learning with Computer Simulation (ILCS)

S A Amalia, E Suhendi, I Kaniawati, A Samsudin, N J Fratiwi, S R Hidayat, A Zulfikar, F N Sholihat, D S Jubaedah, A H Setyadin, M G Purwanto, M H Muhaimin, S S Bhakti and N F Afif

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Distribution of Magnetic Susceptibility of Natural Iron Sand in the Sarmi Coast Area

O Togibasa, M Akbar, A Pratama and S Bijaksana

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Heart Sounds Determination Based on Sliding Window Maximum Method

Bintang Adi Kusuma, Nuryani Nuryani and Darmanto

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OPEN ACCESS 012076

The Effect of Microwave Duty Cycle on The Electrical Conductivity of Reduced Graphene Oxide (rGO)

Utiya Hikmah, Erythrina Stavila, Dadang Suhendar, Akfiny Hasdi Aimon and Ferry Iskandar

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Magnetic characterization of industrial dust from Gresik, East Java, Indonesia

T Lestyowati, S J Fajar and S Bijaksana

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Magnetic characterization of pyroclastic density current (PDC) of the A.D. 1257 eruption of Mt. Samalas, Lombok, Indonesia: preliminary results

A Wijaya, S J Fajar and S Bijaksana

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A Comparative Study of Simulated Annealing and Genetic Algorithm Method in Bayesian Framework to the 2D-Gravity Data Inversion

A.S. Putra, Sukono, W. Srigutomo, Y. Hidayat and E. Lesmana

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Realization of Null-type Bridge Instrument to Determine Water Level to Anticipate Flood Using Inquiry-based Learning

Mohamad Reza Nurrahman, Andi Gumarilang Cakti, Kevin Misrano, Elfi Yuliza and and Khairurrijal Khairurrijal

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The Physical Mechanisms of Geothermal Reservoir During Hydraulic Injection Through Microearthquake Tomography

K A Natania, D P Sahara, A D Nugraha and I. Ramadhan

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Magnetic characterization and heavy metals pollutions of sediments in Citarum River, Indonesia

S Sudarningsih, H Aliyah, S J Fajar and S Bijaksana

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The Recent Small Earthquakes around Lembang Fault, West Java, Bandung, Indonesia

A D Nugraha, P Supendi, B S Prabowo, S Rosalia, Erlangga, Y M Husni, S Widiyantoro, N T Puspito and A Priyono

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The pattern of local stress heterogeneities along the central part of the Great Sumatran fault: A preliminary result

David P. Sahara and Sri Widiyantoro

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Stress drop, earthquake aftershocks and regional stress relation based on synthetic static Coulomb failure stress model

D Kusumawati, D P Sahara, A D Nugraha and N T Puspito

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OPEN ACCESS 012093

A Facile Microwave-Assisted Synthesis of Carbon Dots and Their Application as Sensitizers in Nanocrystalline TiO_2 Solar Cells

I Alkian, A Prasetio, L Anggara, Karnaji, M H Fonisyah, Z M Rizka and H Widiyandari

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OPEN ACCESS 012094

Utilization of Double-Difference Tomography for Geothermal Exploration: 3D Velocity Structure Interpretation and Fluid Determination

A Hijriani, D P Sahara, A D Nugraha, I Ramadhan and R P Sidik

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3D Seismic Tomography to Image the Subsurface Structure of "IY" Geothermal Field Using Double-Difference Method and Waveform Cross-Correlation: Preliminary Results

Indriani Yunitasari, Andri Dian Nugraha and Mohammad Rachmat Sule

+ View abstract View article PDF

OPEN ACCESS 012096

Implementation of GMSTech – a New Practical Software for Microseismic Data Processing – for Estimating Event Source Parameters

Rexha V Ry, D P Sahara, M Rohaman, C Suhendi, K H Palgunadi, S Widiyantoro, A D Nugraha, T Yudistira, B S Prabowo and B Mujihardi

+ View abstract View article PDF

OPEN ACCESS 012097

Review of Progress in Magnetorotational Instability

Himawan Winarto

+ View abstract View article PDF

OPEN ACCESS 012098

Development of Brewster angle measurement instrument using microcontroller unit

Ahmad Marzuki, Lintang Bongkar Girana, Mahmudah Salwa Gianti and Fendi Aji Purnomo

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OPEN ACCESS 012099

Western Java Ambient Noise Tomography: A Preliminary Result

Shindy Rosalia, Sri Widiyantoro, Tedi Yudistira, Phil Cummins and Andri Dian Nugraha

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Investigation on 3D Fractal Dimension as Complexity Parameter of Interconnected Pore in 3D Porous Media

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Self-Similarity Investigation on 3D Pigeon-hole Model as 3D Fractal Rock Model

A K Rochmatulloh, U Z Fawziah, S Feranie and F D E Latief

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Field Localization for the 5-Dimensional Nonminimal Derivative Coupling of The Scalar Field with Modified Randall-Sundrum Model

M R Taufani, A Suroso and F P Zen

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Design Of Microtremor Monitoring Tools Using Accelerometer Sensor On Android Mobile To Determine The Natural Building Frequency In UNS Library

Rio Riantana, Darsono and Agus Triyono

+ View abstract View article PDF

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Pre-service Science Teachers' Conceptual Understanding of Integrated Science Subject: A Case Study

N Winarno, A Widodo, D Rusdiana, D Rochintaniawati and R M A Afifah

+ View abstract View article PDF

OPEN ACCESS 012105

Shifting from physics teacher to basic-science teacher: adequate or not? (a self-study)

Regina Lichteria Panjaitan

+ View abstract View article PDF

OPEN ACCESS 012106

Modeling geomechanical responses induced by CO2 injection in CCS pilot project in Gundih field, Indonesia

Fatkhan, Cahli Suhendi, David P Sahara and Mohammad Rachmat Sule

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Electronic Structure Calculations of Alkali Lead Iodide $APbI_3$ (A=Li, Na, K, Rb or Cs) using Density Functional Theory (DFT) Method

P Pitriana, T D K Wungu, H Herman and R Hidayat

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The Effect of Earthquake to Stability and Run Out Distance of Landslide During Rainfall : a case study of landslide prone area in West Java, Indonesia

C Rizkianti, S Feranie and A Tohari

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Chitosan Nanoparticle-Based Coating as Post-harvest Technology in Banana

Rizkita Rachmi Esyanti, Herafi Zaskia, Annisa Amalia and dan Husna Nugrahapraja

+ View abstract View article PDF

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Canonical Quantization of Geometrized Mechanics

David Senjaya and Jusak Sali Kosasih

+ View abstract View article PDF

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Experiments on Natural Convection as Cooling System Mechanism on Nuclear Reactors

Habibi Abdillah and A Novitrian

+ View abstract View article PDF

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RHEED patterns of 3 nm carbon layer coated Si(111) surface using Sputtering

R Suryana, D K Sandi, H Nakahara and Y Saito

+ View abstract View article PDF

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Pressure Mapping System Development Based on Intensity Modulated Fiber Sensor

A Marzuki, M S Gianti, L B Girana, H Purwanto and S A Kristiawan

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+ View abstract View article PDF

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Local existence of scalar wave equation on the Robertson-Walker universe as a background with $k = 0$

M. Iqbal, F. T. Akbar and B. E. Gunara

+ View abstract View article PDF

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Plutonium and Minor Actinides Utilization in FUJI-U1 Molten Salt Reactor

Cici Wulandari, Abdul Waris, Sidik Permana and Syeilendra Pramuditya

+ View abstract View article PDF

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Homogenous (Th,Pu)O_2 Fuel Utilization on High Temperature Test Reactor 30MWt

Anni Nuril Hidayati, Abdul Waris, Dwi Irwanto and Asril Pramutadi

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HTTR 30MWth Reactor with Homogenous (Th,U)O_2 Fuel

Anni Nuril Hidayati, Abdul Waris, Dwi Irwanto and Asril Pramutadi

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Advanced Nuclear Reactor AP1000 with ThO_2-UO_2 Fuel

R.F. Baskara, A. Waris, R. Kurniadi, K. Basar, Widayani and S. Sahin

+ View abstract View article PDF

Table of contents

Volume 1204

April 2019

Previous issue Next issue

7th Asian Physics Symposium 29–31 August 2017, Bandung, Indonesia

Accepted papers received: 05 March 2019
Published online: 07 May 2019

View all abstracts

Preface

Papers

OPEN ACCESS 012025

Effect of Higher Order Thinking Virtual Laboratory (HOTVL) in Electric Circuit on Students' Creative Thinking Skills

S Sapriadil, A Setiawan, A Suhandi, A Malik, D Safitri, S A S Lisdiani and N Hermita

+ View abstract View article PDF

OPEN ACCESS 012026

Reducing Eleventh-Grade Students' Misconceptions on Gravity Concept using PDEODE ∗E-Based Conceptual Change Model

A Zulfikar, D Saepuzaman, H Novia, A H Setyadin, D S Jubaedah, F N Sholihat, M H Muhaemin, N F Afif, N J Fratiwi, S S Bhakti, S A Amalia, S R Hidayat, Z Nursani, N Hermita, B Costu and A Samsudin

+ View abstract View article PDF

OPEN ACCESS 012027

Optimizing Students' Conceptual Understanding on Electricity and Magnetism through Cognitive Conflict-Based Multimode Teaching (CC-BMT)

A Samsudin, A Suhandi, D Rusdiana, I Kaniawati, N J Fratiwi, A Zulfikar, M H Muhaemin, N Hermita, Mansur, F C Wibowo, Supriyatman, A Malik and B Costu

+ View abstract View article PDF

OPEN ACCESS 012028

Enthalpy of Formation of Na_xCoO_2 and $(Na, Mg)_xCoO_2$ Systems: A First Principle Calculation Study

Ivan Kurniawan and Bambang Prijamboedi

+ View abstract View article PDF

OPEN ACCESS 012029

Phenomenology of Minimal Composite Double Higgs Model

Bayu Adi Nugraha Putra and Jusak Sali Kosasih

+ View abstract View article PDF

OPEN ACCESS 012030

Characterization of Calcium Powders from Merauke Mangrove Crab Shells

K Dahlan, E Haryati, O Togibasa and K Dahlan

+ View abstract View article PDF

OPEN ACCESS 012031

Protein and Minerals Analyses of Mangrove Crab Shells (*Scylla serrata*) from Merauke as a Foundation on Bio-ceramic Components

E Haryati, K Dahlan, O Togibasa and K Dahlan

+ View abstract View article PDF

OPEN ACCESS 012032

Characterization of Tartaric-Sulphuric Acid Anodized 2024-T3 Aluminium Alloys with Anodizing Potential Variation

M H Setianto and Akhmad A. Korda

+ View abstract View article PDF

OPEN ACCESS 012041

Preliminary Study on Electrical Properties of Hydrocarbon-Contaminated Soils at an Artisanal Oil Field in Central Java, Indonesia

E. Agustine, I D Dimawani, D. Fitriani, T D Pambudi, W. Srigutomo, S J Fajar and Trimadona

+ View abstract View article PDF

OPEN ACCESS 012042

Excavating the Quality of Vocational Students' Mental Models and Prediction on Heat Conduction

I M Sari, D Fauzi, A Malik, D Saepuzaman, T R Ramalis and D Rusdiana

+ View abstract View article PDF

OPEN ACCESS 012043

3-D Modeling of Time Domain Electromagnetic (TDEM) Method to Analyze the Layered Earth Structure in the Geothermal Systems

Cahyo Aji Hapsoro, Wahyu Srigutomo and Acep Purqon

+ View abstract View article PDF

OPEN ACCESS 012044

The Field Localization of Yukawa Interaction in a Modified Randall-Sundrum Model

Dewi Wulandari, Triyanta, Jusak S. Kosasih and Douglas Singleton

+ View abstract View article PDF

OPEN ACCESS 012045

Enhancing Junior High School Students Conceptual Understanding Using the POE-based Demonstration Technique on Electrostatics

M G Purwanto, S R Hidayat, N J Fratiwi, A Zulfikar, M H Muhaimin, S S Bhakti, F N Sholihat, A H Setyadin, D S Jubaedah, S A Amalia, N F Afif, A Sutiadi, N Hermita and A Samsudin

+ View abstract View article PDF

OPEN ACCESS 012046

Promoting Oral-Communication Skill to the students of Seventh Grade on Earth Science Content Using Multimedia Based Integrated Instruction (MBI_2)

A H Setyadin, S R Hidayat, S S Bhakti, A Zulfikar, N J Fratiwi, M H Muhaimin, S A Amalia, D S Jubaedah, F N Sholihat, M G Purwanto, N F Afif, D T Chandra, P Siahaan, E Suhendi, I Kaniawati and A Samsudin

+ View abstract View article PDF

OPEN ACCESS 012047

Hexagonal close-packed stability in two-dimensional selfgravitation granular particles system

P M Widartiningsih, S N Khotimah, B Dermawan and S Viridi

+ View abstract View article PDF

OPEN ACCESS 012048

Constructing Essay Questions To Assess Scientific Creative And Critical Thinking Simultaneously Related To Collision Problem Based On Students Responses

Iyon Suyana, Sarah Nadaipah, Parlindungan Sinaga and Selly Feranie

+ View abstract View article PDF

OPEN ACCESS 012049

Analyzing Students Responses To Construct Open Ended Question To Assess Scientific Creative And Critical Thinking (SCCT-Test) Related To Hydrostatic Pressure

H Rusnayati, N Oktavianti, H Novia, D Saepuzaman and S Feranie

+ View abstract View article PDF

OPEN ACCESS 012050

Geomagnetic Map of Field Camp Geophysics in Karangsambung using Data Acquisition 2005-2017

Eko Januari Wahyudi and Dedi Sukmayadi

+ View abstract View article PDF

OPEN ACCESS 012051

Antibacterial Investigation Activity of Titania Anatase technical grade on polypropylene sheet

D O Margaretta, K W Permadi, D Y Rahman, F D Utami, S Viridi and M Abdullah

+ View abstract View article PDF

OPEN ACCESS 012052

Calculation of the binding energy of the lithium nucleus with the yukawa potential and the hellmann potential using WKB approximation

Ahmad Suaif, Dina Rahmawati and Zaki Su'ud

+ View abstract View article PDF

OPEN ACCESS 012053

The Effect of Hydrophilic Coating on Concrete Pile Surface in Pile Driving: Field Test

Nadya Amalia, Elfi Yuliza, Mamat Rokhmat, Edy Wibowo, Sparisoma Viridi and Mikrajuddin Abdullah

+ View abstract View article PDF

OPEN ACCESS 012054

Engaging Students in STEM Based Learning Through Media and Technology

I R Suwarma, I Kaniawati and D S Kaniawati

+ View abstract View article PDF

OPEN ACCESS 012055

Thermophysical parameters of organic PCM coconut oil from the T-history method and its variation with the chemical dopant

Alfriska O Silalahi, I M Sutjahja, D Kurnia and S Wonorahardjo

+ View abstract View article PDF

OPEN ACCESS 012056

The role of particle dopant to the thermal conductivities of PCM coconut oil by means of the T-history method

I M Sutjahja, Alfriska O Silalahi, D Kurnia and S Wonorahardjo

+ View abstract View article PDF

OPEN ACCESS 012057

The enthalpy-temperature curve of new PCM $Ca(NO_3)_2.4H_2O$ and $Co(NO_3)_2.6H_2O$ for low-temperature latent TES

Alfriska O Silalahi, I M Sutjahja, D Kurnia and S Wonorahardjo

+ View abstract View article PDF

OPEN ACCESS 012058

Identifying pre-service physics teacher mental model on electric conceptions

Supriyatman, Andi Suhandi, Dadi Rusdiana, Achmad Samsudin and Firmanul C. Wibowo

+ View abstract View article PDF

OPEN ACCESS 012059

Thermal Effect on Electromagnetic Suspension for Air Gap Performance in Magnetic Levitation System

Deny Viviantoro, Aliq Zuhdi, Agus Purbhadi and Mujamilah

+ View abstract View article PDF

OPEN ACCESS 012060

The development of higher order thinking laboratory (hotlab) model related to heat transfer topic

A Malik, A Setiawan, A Suhandi, A Permanasari, A Samsudin, Y Dirgantara, H Y Suhendi, I M Sari and N Hermita

+ View abstract View article PDF

OPEN ACCESS 012061

Radiation shielding design of neutron source from Kartini reactor's beam-port for SAMOP test facility

Tegas Sutondo and Syarip

+ View abstract View article PDF

Syuhada Syuhada, Nanang Tyasbudi Puspito, Titi Anggono, Nugroho Dwi Hananto, Hendra Grandis and Tedi Yudistira

+ View abstract View article PDF

OPEN ACCESS 012070

Geochemical Characteristics of Volcanic Rocks from Mt. Masurai's Caldera, Jambi, Indonesia

Asep Rohiman, Dipowiguno Prijanto, Arief Prabowo, Antonius Ratdomopurbo, Ruly Setiawan, Mutiara Effendi and Eko Wahyudi

+ View abstract View article PDF

OPEN ACCESS 012071

Myocardial infarction detection system from PTB diagnostic ECG database using Fuzzy inference system for S-T waves

A N Ardan, Miftahul Ma'arif, Z H Aisyah, M Olivia and S M Titin

+ View abstract View article PDF

OPEN ACCESS 012072

Optimalization of ultrasonic tomography method using robotic instrument

Tedy Setiawan, Fatkhan, Fernando Lawrens and Albertus Ariel Rahadi

+ View abstract View article PDF

OPEN ACCESS 012073

Diagnosis of Student's Misconception on Momentum and Impulse Trough Inquiry Learning with Computer Simulation (ILCS)

S A Amalia, E Suhendi, I Kaniawati, A Samsudin, N J Fratiwi, S R Hidayat, A Zulfikar, F N Sholihat, D S Jubaedah, A H Setyadin, M G Purwanto, M H Muhaimin, S S Bhakti and N F Afif

+ View abstract View article PDF

OPEN ACCESS 012074

Distribution of Magnetic Susceptibility of Natural Iron Sand in the Sarmi Coast Area

O Togibasa, M Akbar, A Pratama and S Bijaksana

+ View abstract View article PDF

OPEN ACCESS 012075

Heart Sounds Determination Based on Sliding Window Maximum Method

Bintang Adi Kusuma, Nuryani Nuryani and Darmanto

+ View abstract View article PDF

OPEN ACCESS 012076

The Effect of Microwave Duty Cycle on The Electrical Conductivity of Reduced Graphene Oxide (rGO)

Utiya Hikmah, Erythrina Stavila, Dadang Suhendar, Akfiny Hasdi Aimon and Ferry Iskandar

+ View abstract View article PDF

OPEN ACCESS 012077

Magnetic characterization of industrial dust from Gresik, East Java, Indonesia

T Lestyowati, S J Fajar and S Bijaksana

+ View abstract View article PDF

OPEN ACCESS 012078

Magnetic characterization of pyroclastic density current (PDC) of the A.D. 1257 eruption of Mt. Samalas, Lombok, Indonesia: preliminary results

A Wijaya, S J Fajar and S Bijaksana

+ View abstract View article PDF

OPEN ACCESS 012079

A Comparative Study of Simulated Annealing and Genetic Algorithm Method in Bayesian Framework to the 2D-Gravity Data Inversion

A.S. Putra, Sukono, W. Srigutomo, Y. Hidayat and E. Lesmana

+ View abstract View article PDF

OPEN ACCESS 012080

Realization of Null-type Bridge Instrument to Determine Water Level to Anticipate Flood Using Inquiry-based Learning

Mohamad Reza Nurrahman, Andi Gumarilang Cakti, Kevin Misrano, Elfi Yuliza and and Khairurrijal Khairurrijal

+ View abstract View article PDF

OPEN ACCESS 012081

The Physical Mechanisms of Geothermal Reservoir During Hydraulic Injection Through Microearthquake Tomography

K A Natania, D P Sahara, A D Nugraha and I. Ramadhan

+ View abstract View article PDF

OPEN ACCESS 012082

Magnetic characterization and heavy metals pollutions of sediments in Citarum River, Indonesia

S Sudarningsih, H Aliyah, S J Fajar and S Bijaksana

+ View abstract View article PDF

OPEN ACCESS 012083

The Recent Small Earthquakes around Lembang Fault, West Java, Bandung, Indonesia

A D Nugraha, P Supendi, B S Prabowo, S Rosalia, Erlangga, Y M Husni, S Widiyantoro, N T Puspito and A Priyono

+ View abstract View article PDF

The pattern of local stress heterogeneities along the central part of the Great Sumatran fault: A preliminary result

David P. Sahara and Sri Widiyantoro

+ View abstract View article PDF

OPEN ACCESS 012092

Stress drop, earthquake aftershocks and regional stress relation based on synthetic static Coulomb failure stress model

D Kusumawati, D P Sahara, A D Nugraha and N T Puspito

+ View abstract View article PDF

OPEN ACCESS 012093

A Facile Microwave-Assisted Synthesis of Carbon Dots and Their Application as Sensitizers in Nanocrystalline TiO_2 Solar Cells

I Alkian, A Prasetio, L Anggara, Karnaji, M H Fonisyah, Z M Rizka and H Widiyandari

+ View abstract View article PDF

OPEN ACCESS 012094

Utilization of Double-Difference Tomography for Geothermal Exploration: 3D Velocity Structure Interpretation and Fluid Determination

A Hijriani, D P Sahara, A D Nugraha, I Ramadhan and R P Sidik

+ View abstract View article PDF

OPEN ACCESS 012095

3D Seismic Tomography to Image the Subsurface Structure of "IY" Geothermal Field Using Double-Difference Method and Waveform Cross-Correlation: Preliminary Results

Indriani Yunitasari, Andri Dian Nugraha and Mohammad Rachmat Sule

+ View abstract View article PDF

OPEN ACCESS 012096

Implementation of GMSTech – a New Practical Software for Microseismic Data Processing – for Estimating Event Source Parameters

Rexha V Ry, D P Sahara, M Rohaman, C Suhendi, K H Palgunadi, S Widiyantoro, A D Nugraha, T Yudistira, B S Prabowo and B Mujihardi

+ View abstract View article PDF

OPEN ACCESS 012097

Review of Progress in Magnetorotational Instability

Himawan Winarto

+ View abstract View article PDF

OPEN ACCESS 012098

Development of Brewster angle measurement instrument using microcontroller unit

Ahmad Marzuki, Lintang Bongkar Girana, Mahmudah Salwa Gianti and Fendi Aji Purnomo

+ View abstract View article PDF

OPEN ACCESS 012099

Western Java Ambient Noise Tomography: A Preliminary Result

Shindy Rosalia, Sri Widiyantoro, Tedi Yudistira, Phil Cummins and Andri Dian Nugraha

+ View abstract View article PDF

OPEN ACCESS 012100

Investigation on 3D Fractal Dimension as Complexity Parameter of Interconnected Pore in 3D Porous Media

UZ Fawziah, AK Rochmatulloh, S Feranie, PFL Tobing and FDE Latief

+ View abstract View article PDF

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Self-Similarity Investigation on 3D Pigeon-hole Model as 3D Fractal Rock Model

A K Rochmatulloh, U Z Fawziah, S Feranie and F D E Latief

+ View abstract View article PDF

OPEN ACCESS 012102

Field Localization for the 5-Dimensional Nonminimal Derivative Coupling of The Scalar Field with Modified Randall-Sundrum Model

M R Taufani, A Suroso and F P Zen

+ View abstract View article PDF

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Rio Riantana, Darsono and Agus Triyono

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N Winarno, A Widodo, D Rusdiana, D Rochintaniawati and R M A Afifah

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P Pitriana, T D K Wungu, H Herman and R Hidayat

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C Rizkianti, S Feranie and A Tohari

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+ View abstract View article PDF

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David Senjaya and Jusak Sali Kosasih

+ View abstract View article PDF

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Experiments on Natural Convection as Cooling System Mechanism on Nuclear Reactors

Habibi Abdillah and A Novitrian

+ View abstract View article PDF

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R Suryana, D K Sandi, H Nakahara and Y Saito

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Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Abstract. In this present work, we calculated two frontier orbital energies - singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) - of dehydrogenated tetrahydrocurumin (THC) using density-functional theory (DFT) in gas phase. We used the energy difference of SOMO and LUMO to assess the stability of dehydrogenated THC after performing a hydrogen atom transfer toward reactive oxygen species (ROS). We began by optimizing dehydrogenated THC at six hydrogen abstraction sites. Two hydrogen abstraction sites are at O-H groups and four hydrogen abstraction sites are at C-H groups. Then, we compared the value of SOMO and LUMO energy difference in each site. Our calculations showed that dehydrogenated THC at O-H groups are more stable than dehydrogenated THC at C-H groups.

1. Introduction

Hydrophilic reactive oxygen species (ROS) is able to penetrate into phospholipid bilayer membrane and oxidizes the membrane [1,2] by abstracting a hydrogen atom. This abstraction process marks the beginning of oxidation chain called lipid peroxidation. Since cell membrane is the outermost part of a cell that protects its organelles, oxidation by ROS may lead to pores formation on the membrane [3] and eventually to a cell degradation.

In order to delay or prevent this oxidation process, one can introduce a molecule that performs antioxidant activity which is the ability to transfer hydrogen atom toward ROS to break an oxidation chain[4,5]. An electron paramagnetic resonance study has shown that tetrahydrocurcumin (THC) molecule possesses slightly better antioxidant activity than its former, curcumin molecule [6]. THC also performs an inhibitory effect on membrane lipid peroxidation, experimentally [7].

Since THC can possibly perform its antioxidant activity by transfering a hydrogen atom, the aim of our research is to calculate the energy difference between frontier orbitals of dehydrogenated THC (dehydrogenated THC is THC that has transferred its hydrogen atom) in gas phase, theoretically. We use density functional theory (DFT) to evaluate two frontier orbital energies of dehydrogenated THC, which are singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) energies. The energy difference between SOMO and LUMO will help us to assess the most possible site in THC that is responsible for antioxidant activity of the molecule, which is the dehydrogenated THC with the highest energy difference in its frontier orbitals.

2. Computational details

THC performed its antioxidant activity by transferring one of its hydrogen atom. In this research, we chose six representative X-H sites that were capable of transferring a hydrogen atom (see figure 1). To calculate the energy difference between frontier orbitals of dehydrogenated THC, we conducted our research in the following steps. First step, we built a dehydrogenated THC by abstracting a hydrogen atom from each X-H sites. Each THC with one less hydrogen atom was called dehydrogenated THC 1, dehydrogenated THC 2, etc. Dehydrogenated THC 2 and dehydrogenated THC 5 were produced as a result of a hydrogen atom abstraction from an O-H groups. While other dehydrogenated THCs were produced as a result of a hydrogen atom abstraction from a C-H groups. Although experimental result has suggested that O-H groups played an important role in hydrogen atom transfer [8], we propose to consider the presence of C-H bonds as well in this research. Our molecule of interest has a symmetrical shape. This means if we draw a line at the center of the molecule, the line will divide the molecule into two equal parts. Thus, among the six representative sites chosen, site 1 was in the same position as site 6, site 2 was in the same position as site 5 and site 3 was in the same position as site 4.

Second step, after building six dehydrogenated THCs, we performed full geometry optimisation using UM05-2X functional and 6-31++G(d,p) basis set. M05-2X functional was chosen because it has been recommended for thermochemistry calculations by its developer [9]. We used an unrestricted calculation (symbolled by letter U) since dehydrogenated THC has lost one electron during the hydrogen abstraction so we treated it as an open shell calculation. The geometry optimisation was calculated using DFT applied in Gaussian 09 suite program [10] in gas phase at 298.15 K. At this step, our calculation produced the frontier orbital energies.

Our last step is to find the energy difference between two frontier orbital energies, which are SOMO and LUMO energies at each dehydrogenated THC.

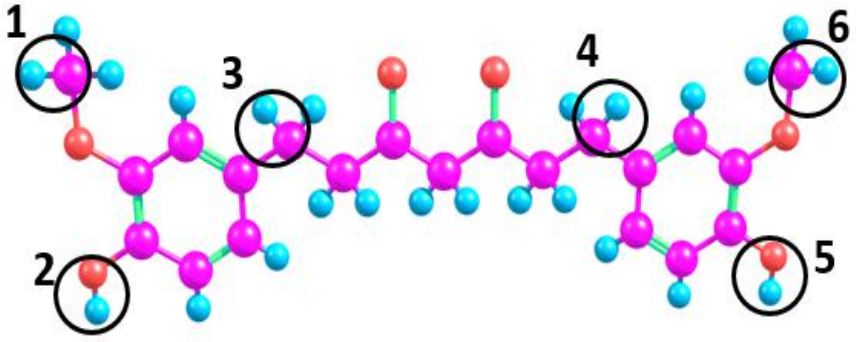

Figure 1. Six representative X-H sites (Blue, pink and red represent H, C and O atoms sequentially). Site 1, 3, 4 and 6 are C-H groups while site 2 and 5 are O-H groups.

3. Results and discussion

Figure 2 showed how model of dehydrogenated THC 2 was built. We built other dehydrogenated THCs with the same procedure. Since dehydrogenated THC 2 has lost one of its electron and proton (recall that we have abstracted a hydrogen atom from THC), we performed geometry optimisation by setting the spin multiplicity into 2 to make sure that the dehydrogenated THC 2 as well as other dehydrogenated THCs were at doublet state.

Figure 3 illustrated the SOMO and LUMO profiles of dehydrogenated THC 2. The SOMO profile was located at the hydrogen transferring sites. The profile informed us the location with the possibility of transferring electrons. After abstracting one hydrogen atom which contains of one proton and one electron, THC molecule was left with only one electron in its last occupied orbital. Thus this orbital was called SOMO. Differ from SOMO profile, LUMO profile was located at the center of the molecule. This profile informed us about the area possible of receiving electrons. Generally, SOMO profiles of all six dehydrogenated THCs were located at transferring sites while their LUMO profiles were located at the center of the molecule.

Our DFT calculation produced many orbital energies of dehydrogenated THCs. We chose two frontier orbitals, SOMO and LUMO, to assess the stability of dehydrogenated THCs[11]. Low energy difference between SOMO and LUMO meant an electron can easily be excited from its ground state, thus a molecule was less stable. While high energy difference between SOMO and LUMO meant an electron can be more stable in its ground state, thus a molecule was more stable.

We calculated energy difference between SOMO and LUMO, which we called it as relative SOMO-LUMO energies, of all six dehydrogenated THCs and tabulated the value in the graph at figure 4. The value of relative SOMO-LUMO energies at dehydrogenated THC 1 (site 1) and dehydrogenated THC 6 (site 6) was almost similar. Their difference was less than 0.2 eV. However, the value are very similar at dehydrogenated THC 2 (site 2) and dehydrogenated THC 5 (site 5), as well as at dehydrogenated THC 3 (site 3) and dehydrogenated THC 6 (site 6). The value of relative SOMO-LUMO energies from the highest to the lowest is dehydrogenated THC 2 = dehydrogenated THC 5 > dehydrogenated THC 1 > dehydrogenated THC 6 > dehydrogenated THC 3 = dehydrogenated THC 4. These results implied that dehydrogenated THC 2 was as stable as dehydrogenated THC 5. Both dehydrogenated THCs were the most stable among all six dehydrogenated THCs. Dehydrogenated THC 1 and 6 were less stable while dehydrogenated THC 3 and 4 had the lowest stability. Based on THC's similarity, site at the same position, possessed similar characters.

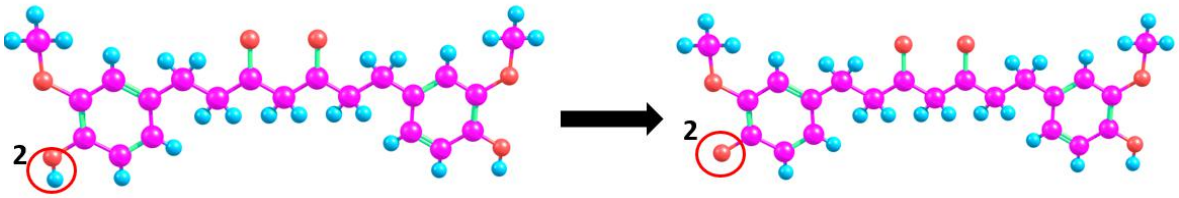

Figure 2. Model of dehydrogenated THC 2

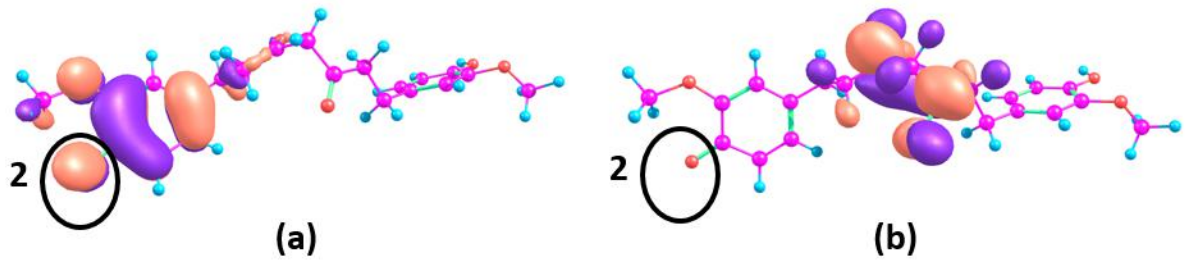

Figure 3. (a) SOMO and (b) LUMO profiles of dehydrogenated THC 2.

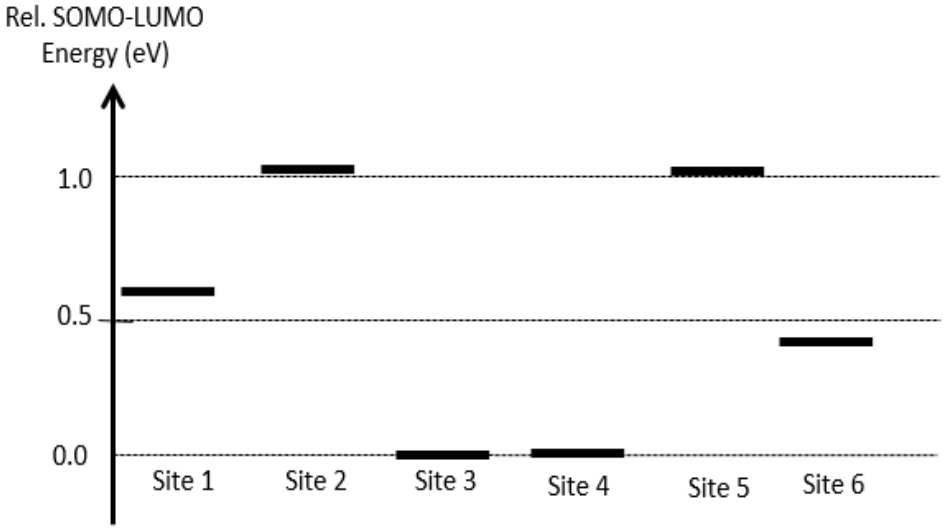

Figure 4. Relative energy diagram of dehydrogenated THC. X axes of the graph is the type of dehydrogenated THC while Y axes of the graph shows the energy difference between SOMO and LUMO.

Finally, in order to assess the most possible site in THC that was responsible for antioxidant activity of the molecule, we concluded the following information. To perform its antioxidant activity, THC should be able to transfer one of its hydrogen atom toward ROS. If the hydrogen atom transferred was originally from an O-H groups, after the transfer process dehydrogenated THC formed would be the most stable. This occured in the case of dehydrogenated THC 2 and 5. However, if the hydrogen atom transferred was originally from a C-H groups, after the transfer process dehydrogenated THC formed would be less stable. This occured in the case of dehydrogenated THC 1, 3, 4 and 6. After performing its antioxidant activity, THC should be able to maintain its stability. Thus the most possible site that is responsible for this activity is O-H groups of THC molecule.

4. Conclusion

We have performed DFT calculation to calculate frontier orbitals of six dehydrogenated THCs. We investigated two frontier orbitals of dehydrogenated THCs, SOMO and LUMO, to assess the stability of the molecules. We suggested that in performing its antioxidant activity, hydrogen atom transfer should occur from O-H groups of THC, since the dehydrogenated THC formed was the most stable. Thus, O-H groups were responsible for the antioxidant activity of THC. This conclusion was supported by our results in two previous researches [12-13].

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