International Conference on Computation in Science and Engineering

IOP Conf. Series: Journal of Physics: Conf. Series **1090** (2018) 011001 doi:10.1088/1742-6596/1090/1/011001

PREFACE

The role of computation and simulation to support research activities in sciences and technologies has become more important in recent decades. The International Conference on Computation in Science and Engineering (ICCSE) 2017 has been conducted in Bandung Institute of Technology (ITB) campus, Bandung, Indonesia, on 10-12 July 2017. This conference is organized by Bandung Institute of Technology (ITB, Indonesia) and supported by UIN Sunan Gunung Jati University. This conference aims at summarizing recent research activities relevant to the computation application in science and engineering and facilitate communication among relevant experts.

More than 150 people from Indonesia, Japan, Malaysia, India, Australia, Korea, and some other countries have participated in this conference. About 150 presentations including 9 plenary talks are presented. The presentations are grouped into 12 areas of particular interest: (1): Complex system Modelling, (2): Energy System Computation, (3): Fluid Dynamics Computation, (4): Artificial Intelligent and Soft Computing, (5): High Energy Physics, (6): Simulation in general, (7): Quantum Computation, (8) HPC, (9): Material Computation, (10): Sub surface modelling and computation, (11): Nuclear and Radiation Computation, and (12): Atmospheric and meteorological computation.

From about 100 full papers submitted after the conference for publication in IOP conference proceedings, after peer review process by relevant experts, 83 papers were accepted for publication in this proceeding. We are indebted to all of authors for submitting their original papers.

We would like to thank all participants, all members of the International Board, members of the Organizing Committee, and I express my gratitude to all those who helped the success of this conference.

Zaki Su'ud

ICCSE 2017 Chairman

Dwi Irwanto

ICCSE 2017 Co-Chairman

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Frontier Orbitals of Dehydrogenated Tetrahydrocurcumin in Water Solvent: A Theoretical Study

IOP Conf. Series: Journal of Physics: Conf. Series **1090** (2018) 012029 doi:10.1088/1742-6596/1090/1/012029

Frontier Orbitals of Dehydrogenated Tetrahydrocurcumin in Water Solvent: A Theoretical Study

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Abstract. We studied two frontier orbitals - the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO)- of tetrahydrocurumin (THC) using density-functional theory (DFT) in water solvent. These orbitals were observed in THC molecule without one hydrogen atom (dehydrogenated THC). The loss of hydrogen atom is due to the transfer of the atom from THC molecule toward reactive oxygen species (ROS) (Hydrogen atom transfer –HAT- mechanism). We began our investigation by optimizing dehydrogenated THC at three X-H sites. Then, water solvent was added by using polarized continuum model (PCM) method. This study observed that dehydrogenated THC at two O-H sites has wider gap of HOMO-LUMO compare to C-H site.

1. Introduction

Studying dehydrogenation of THC is an initial step to understand the role of THC as antioxidant based on hydrogen atom transfer (HAT). In biological system, excessive amount of reactive oxygen species (ROS) promotes oxidative stress [1]. Thus, THC is proposed as one of the antioxidant agents that can prevent oxidative stress in biological system. In playing its role, THC is expected to transfer one of its hydrogen atom toward ROS to neutralize the free radical molecule[2]. This is called hydrogen atom transfer mechanism. Due to HAT mechanism, THC is left with one less hydrogen atom or so called dehydrogenated THC. A good antioxidant agent is expected to maintain the stability of its dehydrogenated form[3].

There are two frontier orbitals used to assess stability of dehydrogenated THC. They are the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). Gap between this two orbitals will decide the ability of electrons to jump from HOMO to LUMO. Wide gap means is correlated to high stability while narrow gap is correlated to low stability[4].

In this research, we intend to study two frontier orbitals of THC produced by THC dehydrogenated using first principles. We choose density functional theory (DFT) as our research framework since it can produce frontier orbitals of dehydrogenated THC by constructing electronic structures only. Thus

this is called first principles study. Result of this study will guide us to decide the stability of dehydrogenated THC after transffering a hydrogen atom from an X-H site. We analyze the HOMO and LUMO energy of three X-H sites of THC to lead us to our final conclusion. THC performes better antioxidant reactivity in polar medium [5], so we choose polar water medium as our simulation environment. We are aware of the problematic of PCM in modeling water as solvent in our previous works where the trend predicted by DFT-PCM calculations always break when using water solvent [6,7].

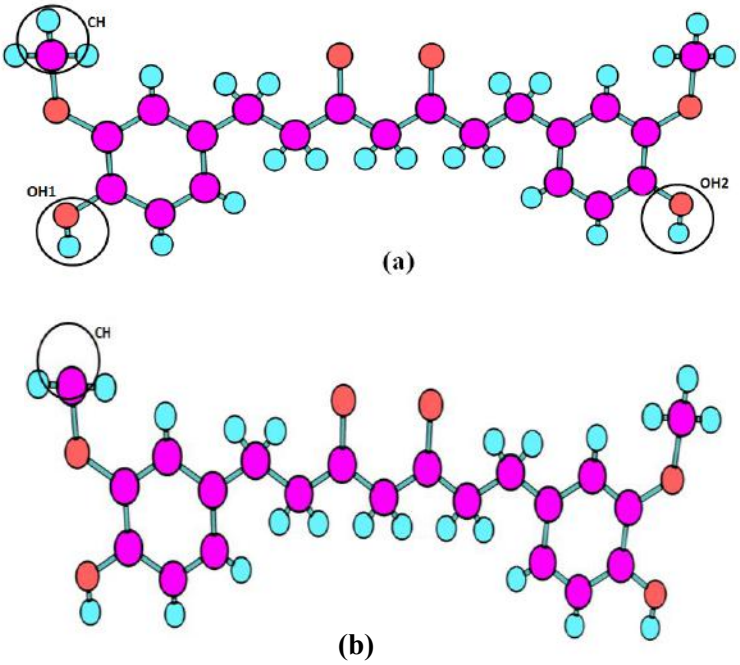

Figure 1. Molecular geometry of (a) THC molecule and (b) dehydrogenated THC produced by abstracting a hydrogen atom from CH site.

2. Computational details

We performed geometry optimization of three THC radicals at site OH1, OH2 and CH using UM05-2X functional and 6-31++G(d,p) basis set. Some authors have successfully used M05-2X functional to study the antioxidant properties of polyphenols [8, 9]. The developer of this functional was also suggesting it for thermochemistry calculations [10]. Since our system was an open shell system of THC dehydrogenated, we performed an unrestricted calculation. Our simulation was done in water environment to represent a polar medium. This solvent effect was included using polarized continuum model (PCM), where water was modelled as cavity that interacts electrostatically with THC radical placed within the cavity [11]. All calculations were performed using Gaussian 09 suite program [12] at 298.15 K.

3. Results and discussion

Figure 1(a) shows model of our molecule of interest which is a THC molecule. Site CH, OH1 and OH2 mark three targeted sites with the ability of transferring a hydrogen atom. We abstract one hydrogen atom from each of this site respectively to create dehydrogenated THC. Figure 1(b) shows

dehydrogenated THC at C-H site. Our DFT calculations coupled with PCM confirms that the geometry of our system is in minimum energy with doublet spin states.

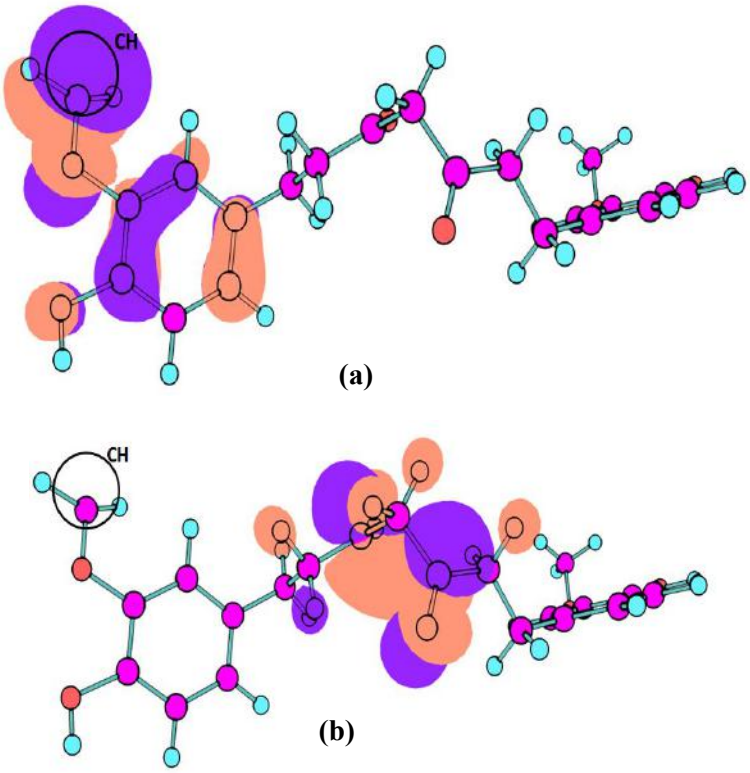

Figure 2. (a) HOMO and (b) LUMO profiles of dehydrogenated THC at CH site.

Figure 2 presents HOMO and LUMO profiles of dehydrogenated THC at C-H site. As shown in 2(a), the HOMO profile is located at dehydrogenated site while in 2(b), the LUMO profile is located in the middle of the molecule. This result is also true for site OH1 and OH2.

Figure 3 summarizes the relative HOMO-LUMO energy of our three dehydrogenated THC systems. In general, O-H sites have higher relative HOMO-LUMO energy than CH site. Higher relative HOMO-LUMO energy means electrons cannot jump easily from HOMO to LUMO. As a result, dehydrogenated THC at O-H sites is more stable than at C-H sites. Site OH1 and OH2 possess very similar value of relative energy HOMO-LUMO. This result predicts that hydrogen atom transfer from both sides will produce the same stability of dehydrogenated THC in water environment. We compare our results to one of our previous work for relative HOMO-LUMO of THC in gas phase [13] and conclude that water solvent does not affect the stability of dehydrogenated THC.

4. Conclusion

The study of frontier orbitals of dehydrogenated THC in water solution showed that when hydrogen atom transfer occured at O-H site, the stability of dehydrogenated THC is higher than when it occured at C-H site. Hydrogen atom transfer at two O-H sites in THC will produce dehydrogenated THC with the same stability.

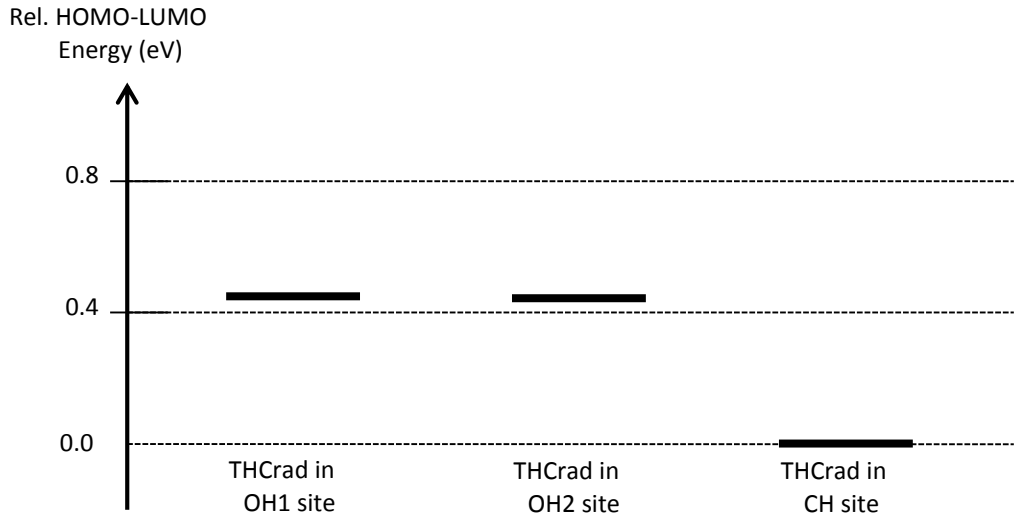

Figure 3. Relative energy diagram of THC radicals in OH1, OH2 and CH sites

Acknowledgement
The authors are grateful to Lembaga Pengelola Dana Pendidikan (LPDP) that has sponsored this research.

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