

**LEMBAR  
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW  
KARYA ILMIAH : PROSIDING**

Judul Karya Ilmiah : Ab Initio Computational Study of electronic structure of -O-C Bonding Formation on Chitosan Polymer-Part 1: Effects of NaOH

Jumlah Penulis : 5 Orang

Status Pengusul : Penulis ke-5

Identitas Prosiding : a. Judul Prosiding : Journal of Physics: Conference Series: The 8<sup>th</sup> Internasional Seminar on New Paradigm and Innovation on Natural Sciences and Its Application (INSPINSA) 2018

b. ISBN/ISSN : 978-1-5108-6265-4 / 1757-8981

c. Thn Terbit, Tempat Pelaks. : 2019, Semarang – Indonesia

d. Penerbit/Organiser : IOP Publishing Ltd

e. Alamat Repository/Web : <https://iopscience.iop.org/issue/1742-6596/1217/1>

Alamat Artikel : <https://iopscience.iop.org/article/10.1088/1742-6596/1217/1/012054>

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- Ruang lingkup dan kedalaman pembahasan:** Artikel ini berisi tentang mekanisme reaksi dari pembentukan ikatan O-C dan membandingkan pengaruh katalis NaOH pada polimer kitosan. Penulis dapat menjelaskan mekanisme pembentukan O-CMC dengan metode komputasi. Penulis dapat membandingkan serta menjelaskan efek penggunaan katalis NaOH dan tanpa katalis pada pembentukan O-CMC. Data yang terdapat pada artikel ini meliputi: sudut ikatan, panjang ikatan, sudut dihedral, energi optimasi, energi gap HOMO-LUMO, dan energi aktivasi. Penulis menggunakan metode komputasi sehingga diperoleh nilai  $\Delta G$  dan  $\Delta H$  yang dapat digunakan untuk mengetahui bahwa reaksi berlangsung secara spontan dan eksotermik. Artikel ini disusun dengan dasar referensi jurnal bereputasi secara sistematis. Penulis mampu menyusun pembahasan secara jelas dan mudah dipahami.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** Informasi dan data yang dipaparkan penulis dalam artikel studi komputasi ini sudah sangat lengkap dan mudah dipahami. Referensi yang digunakan adalah jurnal internasional yang bereputasi. 31 % referensi yang terbit 5 tahun sebelum artikel/jurnal ini terbit.
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Prof. Dr. Meiny Suzery, MS  
NIP. 196005101989032001  
Unit Kerja : Kimia FSM Undip

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- Ruang lingkup dan kedalaman pembahasan:** Penulis membahas mengenai studi komputasi abinitio pembentukan ikatan O-C pada polimer chitosan serta pengaruh katalis NaOH dalam reaksi tersebut. Cakupan yang dibahas dalam artikel di antaranya; mekanisme yang terjadi dalam pembentukan O-CMC dengan katalis dan tanpa katalis. Parameter yang diperhitungkan dalam menentukan reaksi yang paling disukai di antara keduanya adalah panjang ikatan, sudut ikat, sudut dihedral, energi optimasi, energi gap HOMO-LUMO, dan energi aktivasi hingga akhirnya diperoleh laju dari setiap reaksi. Dalam artikel, penulis juga dapat memperoleh nilai  $\Delta G$  dan  $\Delta H$  sehingga mengetahui bahwa reaksi pembentukan O-CMC dapat terjadi secara langsung atau berlangsung secara eksotermis. Penjabaran mekanisme reaksi yang dilakukan oleh penulis dengan kajian ilmu komputasi dapat dijelaskan setiap langkahnya secara lengkap dan urut dan berasal dari jurnal-jurnal yang bereputasi. Pembahasan dalam artikel dilakukan secara sistematis, sehingga dapat digunakan sebagai informasi awal dalam penelitian empiris di laboratorium. Layout tabel 1 bertumpuk dengan naskah sehingga beberapa kalimat tidak terbaca serta tabel 2 tidak disitasi dan dibahas (8)
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Semarang, 26-03-2021

Reviewer 2

A handwritten signature in black ink, consisting of a large, stylized initial 'M' followed by a cursive 'C' and 'D'.

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si

NIP 19700702 199603 1 004

Unit Kerja : Kimia FSM Undip

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Hasil Penilaian *Peer Review* :

Komponen Yang Dinilai	Nilai Reviewer		Nilai Rata-rata
	Reviewer I	Reviewer II	
a. Kelengkapan unsur isi prosiding (10%)	3,00	3,00	3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	8,00	8,00	8,00
c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%)	8,00	8,00	8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	8,50	9,00	8,75
<b>Total = (100%)</b>	<b>27,50</b>	<b>28,00</b>	<b>27,75</b>
<b>Nilai Pengusul = (40% x 27,75 ) = 11,10</b>			

Semarang, 12 April 2023

Reviewer 2



Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si  
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Reviewer 1



Prof. Dr. Meiny Suzery, MS  
NIP. 196005101989032001  
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#### Document type

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#### Source type

Conference Proceedings

#### ISSN

17426588

#### DOI

10.1088/1742-6596/1217/1/012054

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## Ab initio computational study of electronic structure of o-c bonding formation on chitosan polymer-part 1: Effects of NaOH

Yuliani, Shella V.<sup>a</sup>; Salimah S.N.M.<sup>a</sup>; Hudyanti, Dwi<sup>a</sup>; Laksitorini, Marlyn Dian<sup>b</sup>; Sahaan, Parsaoran<sup>a</sup>

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<sup>a</sup> Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia

<sup>b</sup> Department of Pharmaceutics, Faculty of Pharmacy, Gadjah Mada University, Sekip Utara, Yogyakarta, Indonesia

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### Abstract

Carboxymethyl chitosan (CMC) is a biopolymer that has water-soluble properties, high viscosity, biocompatibility, biodegradable, and low toxicity. CMC can be made by direct alkylation using monocloroacetic acid to produce chitosan derivatives under certain reaction conditions with NaOH as a catalyst. This research aims to explain one the reaction mechanism of bonding formation of O-C and to

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compare with the effect of the presence of NaOH as a catalyst. The reaction mechanism of O-CMC formation studied by the computational method. Chitosan polymer is very complex, so the molecule model used for calculation is chitosan dimer segment. The stable molecular structure of chitosan dimer which is involved in the reaction mechanism was optimized using ab initio computational method based on Hartree Fork theory and 6-31G(d,p) basis set. Mechanism of O-CMC synthesis reaction was modeled into  $S_N^2$  reaction (bimolecular nucleophilic substitution) which results in PO-CMC-2. The study showed that the-O-C bonding formation by  $S_N^2$  model and NaOH as a catalyst was more preferred with an activation energy of 323,321  $\text{kJ}\cdot\text{mol}^{-1}$  than without NaOH as a catalyst with an activation energy of 533,22  $\text{kJ}\cdot\text{mol}^{-1}$ . The mechanism of the synthesis reaction of O-CMC is an exothermic reaction and spontaneously. © Published under licence by IOP Publishing Ltd.

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# The 8th International Seminar on New Paradigm and Innovation on Natural Science and Its Application


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Journal of Physics: Conference Series, Volume 1217, The 8th International Seminar on New Paradigm and Innovation on Natural Science and Its Application 26 September 2018, Central Java, Indonesia

**Citation** 2019 *J. Phys.: Conf. Ser.* **1217** 011001**DOI** 10.1088/1742-6596/1217/1/011001

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## Abstract

The 8th International Seminar on New Paradigm and Innovation on Natural Sciences and Its Application (ISNPINSA-8) is annual seminars organized by Faculty of Sciences and Mathematics (FSM) Diponegoro University and has been successfully conducted since 2011. The ISNPINSA-8 was held in Semarang, Indonesia on September 26<sup>th</sup> 2018. The aims of ISNPINSA are to facilitate brain storming and state of the art information in field of sciences and mathematics; to increase innovation of technology that can be applied in industries; to contribute in formulating strategy to increase the role of science for community; and to stimulate collaboration between industries, researchers and government to increase community welfare. The theme of 8<sup>th</sup> ISNPINSA in 2018 is "*Science and Applied Science for Sustainable Development Goals*".

The number of participants of the seminar were 272 including keynote speakers, invited speakers, oral presenters, poster presenters, and non presenters coming from various institutions of various countries, including Japan, Philippines, Thailand, Malaysia, Australia, Bangladesh, China, Kazakhtan, Vietnam

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2019

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Accepted papers received: 27 March 2019

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