PROCEEDING
THE 2\textsuperscript{nd} INTERNATIONAL CONFERENCE ON CHEMICAL SCIENCES (2\textsuperscript{nd} ICCS-2010)
CHEMISTRY GOES GREEN
Yogyakarta, 14-16 October 2010

Drs. Priatmoko, M.S

JURUSAN KIMIA
FAKULTAS MATEMATIKA DAN ILMU PENGETAHUAN ALAM
UNIVERSITAS GADJAH MADA
YOGYAKARTA
2010
EDITOR'S NOTE

Thank God for the publication of the Proceeding of the second International Conference on Chemical Sciences (the 2nd ICCS 2010). In term of the number of participants, the seminar with theme of “Chemistry Goes Green” was a successful one. There were roughly 200 participants in the Seminar.

We really regret for the postponement of the Proceeding due to unpredicted circumstances especially that of Merapi eruption on October-November 2010. However, we do hope that the delay does not affect the authors to do any kind of ensuing activities.

There were initially 5 plenary papers and 177 regular papers presented in the Seminar. Among those presented works, 96 papers were submitted to the Editor in complete format. The Editor together with the Editor of the Indonesian Journal of Chemistry (IJC) nominated 5 of them to be published in July 2011 edition of the Indonesian Journal of Chemistry. The papers chosen to be published in IJC were selected based on the quality and potential to give a significant impact to the development of the chemical sciences.

Based on the contents, the papers appeared in this Proceeding are grouped into five concentrations that are Environmental and Green Chemistry (25 papers), Chemistry in Life Science and Chemical Biology (21 papers), Information Technology in Chemical Sciences and Computational Chemistry (12 papers), Innovation in Material Chemistry, Supramolecular Chemistry and Nanotechnology (20 papers) and Innovation in Methods, Technique and Instrumentation of Analytical Chemistry (18 papers). The distribution of the papers into those areas was more or less comparable. In the process of the publication of this Proceeding, we did our best to edit the papers to match a good standard of scientific publication.

Finally, we are indebted to all parties who helped in preparing the Proceeding. We wish this Proceeding would considerably contribute to the development of chemistry and those related sciences.

Editor in Chief

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MESSAGE
FROM THE CHAIRMAN OF ORGANIZING COMMITTEE

Assalamualaikum Wr.Wb

Dear Distinguished Guests and Conference Participants,

On the behalf of the organizing committee of the second International Conference on Chemical Sciences (the 2nd ICCS 2010), I am very pleased to welcome you all the participants to this high scientific gathering.

The 2nd ICCS 2010 is held by Chemistry Department Faculty of Mathematic and Natural Sciences Gadjah Mada University, to follow the success of the 1st ISSC held in 2007. The conference having main theme "Chemistry Goes Green" is one of the important meetings exclusively dedicated to Chemists, Chemistry, and Chemistry related sciences to be increasingly green by applying the principles of Green Chemistry to all aspects of basic and applied research and education as well as laboratory management. The 2nd ICCS 2010 is featured by key notes addresses, whether given by overseas and national experts, and a number of contributed lectures. Additionally, there is also poster session, and three best posters will be selected for award winners.

In this great chance I would like to express my gratitude for your tremendous effort to be able to take part in this scientific meeting. Special thanks I deliver to the key note speakers giving your time to give speech and the partners sponsoring this activity. Your contributions have make the conference successful.

Finally, I hopeful that these presentations and mutual discussion will stimulate the development of new concepts to benefit society in general and for all mankind. We wish you a great conference.

Wassalamu'alaikum Wr.Wb.

Chairman of the Organizing Committee

Prof. Dr. Endang Tri Wahyuni, M.S.
MESSAGE
FROM THE CHAIRPERSON OF CHEMISTRY DEPARTMENT
FACULTY OF MATHEMATICS AND NATURAL SCIENCES
UNIVERSITAS GADJAH MADA

Assalamualaikum Wr. Wb.

Dear guests,

Welcome to the 2nd ICCS 2010, Yogyakarta, the second International conference organized by Chemistry Department, Universitas Gadjah Mada.

The 2nd ICCS-2010, which is held from October 14-16th, 2010 in Yogyakarta-Indonesia, conducted following the success of 1st ICCS 2007 is a truly good opportunity for academicians, researchers and industrial practices to present their frontier works leading to innovation in chemical sciences for a better life. Wishing you for a great success in this conference, it is our sincere hope that in this scientific occasion you will actively take part in the discussion and be exposed to advance science and technology, which is expected to comply to the world sustainable-green chemistry paradigm.

On behalf of the Chemistry Department we would like to give our warmest welcome again to you all here in Yogyakarta.

Wassalamu’alaikum Wr. Wb.

Chairperson of Chemistry Dept.,

Prof. Drs. Mudasir, M.Eng, Ph.D.
MESSAGE
FROM THE DEAN FACULTY OF MATHEMATICS AND
NATURAL SCIENCES UNIVERSITAS GADJAH MADA

Assalamualaikum Wr. Wb

Dear Distinguished Guests and Conference Participants,

Welcome to the second International Conference on Chemical Sciences (ICCS) 2010, Yogyakarta-Indonesia. On Behalf of the Faculty of Mathematics and Natural Sciences, Universitas Gadjah Mada, Yogyakarta-Indonesia, I am very pleased to welcome you all the participants to this high scientific gathering. It is a great honour that our faculty is, once again, hosting an international conference on Chemical Sciences. I am deeply thankful for your tremendous effort to be able to take part in this scientific meeting. I would also like to express my gratitude to the organizing committee in making the conference successful. Congratulations!

As you know very well, Chemical Sciences have been evolving together with other fields of Sciences to become front runner and keep contributing enormously to the progress of Sciences and Technology. Many novel innovations in chemical sciences are developed and perfected in order to catch up with the latest issues and to formulate the future directions in chemical knowledge, research and education, as well as to help industrial users and community apply various advancements in chemical sciences. The main theme: “Chemistry Goes Green” which has been selected by the organizing committee, in my opinion, is very appropriate with the big role of Chemical Sciences nowadays in many sectors such as ICT, smart material, environmental protection, life sciences and many others.

We believe that this conference will succeed in bringing together researches, academicians and industrial practices to have scientific exchange of information and networking.

Finally, we wish you a great conference and this ICCS-2010, be highly beneficial to the teaching and research in Chemistry Sciences as well as to welfare of the community.

Wassalamualaikum Wr. Wb.

Dean,

Dr. Chairil Anwar
MESSAGE
FROM THE RECTOR UNIVERSITAS GADJAH MADA

Bismillahirrahmaanirraahiim.
Assalamualaikum Wr. Wb.

Dear Distinguished Guests and all the Conference Participants,

I am honoured to be able to welcome all participants to the International Conference of Chemical Sciences (The 2nd ICCS 2010) to Universitas Gadjah Mada (UGM) here in Yogyakarta. I am pleased to see many of you have come to this event, not only from Indonesia but also neighbouring countries such as Malaysia and Philippines.

Allow me to describe a little bit about our university. As the biggest and oldest state-run university, Universitas Gadjah Mada is committed to excellent research and teaching as well as community service. UGM has been recognized in the world for quality in social and cultural sciences. UGM’s committed encompasses many disciplines, including chemistry.

In today’s world, chemistry is an area of study that is very important for human beings as human beings make use much of chemical products in their daily life. Demands are increasing for the application of science of chemistry and they bring with them greater challenges as well. The contributions made by experts who are gathering here are, therefore, required to be able to meet those demands and challenges.

With many scientists, academicians and industrial players from around the globe participating in the conference. I am confident great things will be achieved as you will collectively turn your thoughts to the comprehensive issues facing chemistry in today’s world to improve the better quality of our live. I hope you can also meet the target of achieving green sustainable chemistry.

Finally, I wish you enjoy this conference and have a pleasant stay in Yogyakarta. In addition, you are very welcomed to have a closer look at our campus by visiting each faculty and unit in person. Thank you.

Wassalamu’alaikum Wr.Wb.

Rector,

Prof. Ir. Sudjarwadi, M.Eng., Ph.D.
CONVERSION OF RHODINOL FROM CITRONELLAG OIL TO
CIS AND TRANS-PS EUDOIONONE

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ABSTRACT

Rhodinol as mixture of citronellol and geraniol has been isolated from the trade citronella oil. Geraniol from rhodinol was changed to become pseudoionone (-ionone). The first step was done to chice the trade citronella oil that by using GC and GC-MS to know the content of rhodinol from each trade citronella oil. Then was done the isolation of rhodinol from citronella oil by using fractional distillation with diminishing pressure. Pseudoionone (-ionone) was obtained via the reaction of the geraniol (from rhodinol) with aluminium isopropoxide with aceton, whereas the citronellal not react. The reaction was done along 10 hours with method of reflux with temperature 75 oC. The product that obtained was done the fractional distillation with dimiss pressure. The yield that obtained was yellow liquid and was analysed by using GC-MS. The content of rhodinol that isolated from trade citronella oil was 68.86%. The reaction between the geraniol from the rhodinol and aluminium isopropoxide and aceton yielded the 16.94% cis-pseudoionone and the 30.34% trans-pseudoionone.

Keywords: pseudoionone, rhodinol

INTRODUCTION

Wijesekera (1973) said that, the component of citronellal oil was citronella and geraniol. In spite of this principle component, the citronellal oil (in particular the citronellal oil type Java) there are other components, there are x-pinene, linanil, citronellisacetial, B-camphorin, elemole and geraniol acetate.

Guenther (1950) was explained that these principal components in this citronellal oil can determine the intensity of the fragrant order, the value and the price.

The isolation of citronellal from citronella oil can be conducted by physical and chemical method.

Sastrohamidjojo (1981) isolated citronellal from the citronellal oil by the physical method that was the fractional distillation at reduced pressure, reasonable the chemical method, that was to react with sodium bisulphite. Then the isolation yield of the citronellal was reacted to become the ester compound and others.

To oxidation the alcohol, there are many oxidator can be used for this reaction. It choice these oxidators depend on the direction and the type of alcohol.

The strong oxidator, like potassium permanganate, mangan (IV) oxide, ruthenium tetra oxide can oxide the primer alcohol to become the aldehyde and then to progress to become the carboxylic acid.

R.CH2OH → R.CH0 → R.COOH

The primer alcohol can also been oxidized to become the aldehyde without oxidized to continue to carboxylic acid. That was by catalytic dehydrogenation method. (March, 1985)

The substance that can be used as the catalyst was Cu- chrome, silver and Cu metal, the dehydrogenation after was to the industry scale.

Ketone can also act as the oxidator with there was base. This reaction was known as Oppenura oxidation. That was opposite of Meerwein-Pondorf Verley (March, 1985). The catalyst that much more used was aluminium alkoxide, potassium, sodium and zirconium alkoxide, aluminum and several transition metal complexes can also be used as catalyst (Nancy, 1984). Aluminum tertiar was the reagent that used this design.

The 2D structure and the 3D structure of the trans-pseudoionon and cis-pseudoionon were given below.
EXPERIMENTAL SECTION

Materials
Material: The trade citronellal oil, isopropanol, Mercury (II) chloride, aluminum metal, carbon tetrachloride, sodium chloride, acetone, ethanol, hydrogen chloride 17.5 %, diethyl ether, blue silica gel, sodium sulfate anhydrous, whatman filter paper.

Procedure
The isolation of rhodinol from citronella oil
The isolation of rhodinol from citronella oil was conducted with fractional distillation at reduce pressure. Then it will be obtained three fractions of distillate and then three fraction of distillate was analyzed by using GC-MS. The condition of GC-MS: column type: DB-1, column: 80-250°C, ionization type: El (Electron Impact), detector temperature 270°C, the amount of sample: 0.4 μL.

The preparation of aluminum isopropoxide
To the three necked flask 250 ml that was completed with cobbler, heater, magnetic stirrer and thermometer, was added 75 ml (58.75 g : 0.98 mole) isopropanol, 0.125 g mercury (II) chloride and 6.75 g (0.25 mole) aluminum metal that filled with blue silica gel. This mixture was heated so that boils, was added tetra chloride 1 ml, the mixture change color to become grey and occurred the exhaust of hydrogen. After all hydrogen release, the mixture was refluxed at 80°C temperature for 12 hours so that all aluminum finishes reacting. Then the mixture was fractional distillation reduced pressure at 170°C with 12 mmHg pressure. The distillate that come out in the shape of viscous uncolor distillate was caught in the bottle that closed together and was pressed in the refrigerator. After 4-5 days it was obtained the white crystal and so this determined melting points.

The 3D structure:

The reaction between aluminum isopropoxide and acetone (Doyle and Mungall, 1980)
Rhodinol that contain 63.71% geraniol was taken 61.11 g and added to the three necks flask capacity 500ml that completed with cooler, magnetic stirrer, heater, and thermometer. Then it was added 51 g (0.25 mole) aluminum isopropoxide and 145 g (2.5 mole) acetone. The mixture was refluxed at 75°C for 10 hours using mantle heater. After refluxing finished the mixture was cooled then it was diluted with 200 ml aquadest and nickel with 17.5 % HCl until pH 3-4. The up layer was separated and down layer was extracted with ether. The up layer and the ether layer was mixed. The mixture was washed until neutral. Then it was dried with anhydrous sodium sulfate. The yield was fractional distilled at reduce pressure and the distillate was analyzed by using GC and GC-MS.

RESULTS AND DISCUSSION

The selection of the trade citronella oil.
From the several types of the citronella oils that stay at Yogyakarta market, were taken three types of sample among other things A from Brataco Chemical Shop, B from Juwita Shop Bringharjo Market, and C from Tekun Jaya Market. From analysis of GC-MS was obtained the result (Table 1).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Contents (in %)</th>
<th>Additional compound</th>
<th>Total rhodinol</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>α-pin</td>
<td>citronellal</td>
<td>citronellol</td>
</tr>
<tr>
<td>A</td>
<td>23.42</td>
<td>25.88</td>
<td>2.83</td>
</tr>
<tr>
<td>B</td>
<td>-</td>
<td>22.22</td>
<td>11.90</td>
</tr>
<tr>
<td>C</td>
<td>-</td>
<td>45.65</td>
<td>11.64</td>
</tr>
</tbody>
</table>

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Table 2. The result of fractional distillation at reduce pressure

<table>
<thead>
<tr>
<th>Fraction</th>
<th>Temp/Pressure °C/mmHg</th>
<th>weight (g)</th>
<th>Volume (mL)</th>
<th>Contained (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>citronellal</td>
</tr>
<tr>
<td>1</td>
<td>85-114</td>
<td>9.30</td>
<td>10.5</td>
<td>45.88</td>
</tr>
<tr>
<td>2</td>
<td>122-125</td>
<td>4.71</td>
<td>5.0</td>
<td>48.91</td>
</tr>
<tr>
<td>3</td>
<td>125-127</td>
<td>21.00</td>
<td>27.0</td>
<td>26.12</td>
</tr>
</tbody>
</table>

Figure 1. Chromatogram of B citronella oil

From above data, therefore the sample that selected to the further process. Consecutive this chromatogram from the selected citronella oil.

The isolation of rhodinol

The B citronella oil was fractional distilled at reduce pressure will be obtained three fractional of distillate after it was conducted analyzing by using GC-MS will be obtained the result below (Table 2). This chromatogram and mass spectra from fractional distillation III is displayed in Figure 2.

Figure 2. Chromatogram of distillate fraction III

From the chromatogram of distillate fraction III can be seen there were two peaks that was peak no 5 retention time 9.45 minutes that was the peak from citronellol and geraniol. This mass spectra of 2 peaks is displayed in Figure 3 and 4. From the mentioned spectrum was seen the peak m/z : 156, 138, 123, 109, 95, 81, 69, 55 its fragmentation is presented in Figure 4.

Figure 3. Mass spectra of Peak 5 and its fragmentation

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Figure 4. Mass spectra of Peak 6 and its fragmentation

Prepare of aluminum isopropoxide
From the reaction of aluminum isopropoxide of crystal from weight 44.87 g, white color and melting points 127-130°C.

The reaction between rhodinol with aluminum

From the chromatogram above was looked at two peaks that are peak retention time 14.40 minutes the peak of cis-pseudoionone and peak retention time 13.85 minutes was trans-pseudoionone.

From two mass spectra of cis and trans-pseudoionone were looked at their differences. At cis-pseudoionone appeared the peaks m/z: 177 on (M-15) or (M-CH₃) and the little peak at m/z: 159, precisely for trans-pseudoionone appeared at m/z: 192. Then those other peaks were exactly the same. As follow their fragmentations.

CONCLUSIONS
From the result of research and the discussion, therefore it can be concluded as below:
1. The rhodinol is the mixture of citronellol and geraniol can be isolated from citronellal oil by using the fractional distillation at reduce pressure, obtained the yield with 68.86% purities.
2. Geraniol in rhodinol was reacted with aluminum isopropoxide and acetone to become cis-pseudoionone and trans-pseudoionone. With 16.94% and 30.34% purity respectively.
REFERENCES


