

PROCEEDINGS

National Workshop  
on  
Instrumentation Techniques  
for  
Research in Chemical Sciences  
(WITRCS - 2017)

22-23 December, 2017



Organized by  
Department of Chemistry  
Kanoria Mahila PG Mahavidyalaya  
Jawahar Lal Nehru Marg, *deem*  
Jaipur, Rajasthan **Principal**  
Kanoria PG Mahila Mahavidyalaya  
JAIPUR

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*National Workshop on Instrumentation Techniques for Research in Chemical Sciences*

**Proceedings**

Of the National Workshop on

**Instrumentation Techniques**  
for  
**Research in Chemical Sciences**  
(WITRCS- 2017)

22-23 December, 2017

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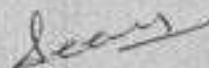
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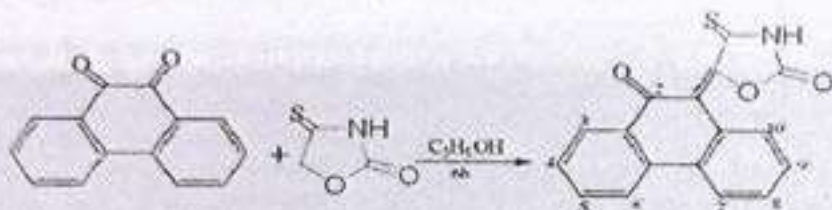
## A one pot synthesis of fused heterocycles

Swati Singh<sup>1</sup> and Sunita Shekhawat<sup>2</sup>

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### Abstract

Fused tri - heterocyclic system have attracted considerable attention due to their potential pharmacological activity and have become valuable alternatives in drug design. For the construction of complex heterocyclic compounds,  $\alpha$ -diketones have assumed much importance because of their multiple reactivity profiles. Phenanthrenequinone derivatives exhibit numerous pharmacological activities like antioxidant, antimalarial, antitumours and antiretroviral. Oxazolidinone, a five membered heterocyclic ring exhibiting potential medicinal properties with preferential antibacterial activity. Scientists reported various synthetic procedures for this heterocyclic structure. Current review articles tried to cover each and every potential aspect of oxazolidinone like synthetic routes, pharmacological mechanism of action, medicinal properties and current research activities. We have carried out the Knoevenagel type condensation reaction of phenanthrenequinone with active methylene heterocycle 2-thioxo-4-oxazolidinone and investigate their configuration by semiempirical methods.



Reaction of phenanthrenequinone with 2-thioxo-4-oxazolidinone

### INTRODUCTION:

Heterocyclic compounds have been a special interest to researchers only in the last 15-20 years.

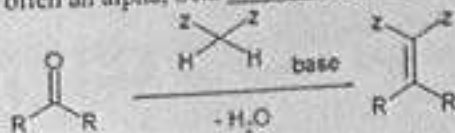
The increased interest in heterocyclic compounds is primarily due to high biological activity of some natural compounds of this group<sup>1-3</sup>. Active methylene heterocycles incorporating toxophores such as and have been reported to possess a wide spectrum of therapeutic activities. Phenanthraquinone derivatives exhibit numerous pharmacological activities like

antioxidant<sup>4</sup>, antimalarial<sup>5</sup>, antitumours and antiretroviral. Therefore, coupling of these two biologically active moieties would be expected to afford interesting series of compounds having enhanced biological properties. So, a good deal of current activity in the sphere of organic chemistry is concerned with the isolation and synthesis of heterocyclic compounds. Over the past hundred years, an increasing volume of research in heterocyclic chemistry has helped to a mass, a vast body of information of interest to organic chemist.

Some heterocycles discovered by Japanese researchers are finding applications in the treatment of carcinomatous diseases and they have a broad spectrum of antibacterial activity, including penicillin and tetracycline<sup>6</sup>.

The **Knoevenagel condensation** reaction is an **organic reaction** named after **Emil Knoevenagel** is a modification of the **Aldol condensation**<sup>7,8</sup>.

A Knoevenagel condensation is a **nucleophilic addition** of an **active hydrogen compound** to a **carbonyl group** followed by a **dehydration reaction** in which a molecule of water is eliminated (hence **condensation**). The product is often an **alpha, beta conjugated enone**.

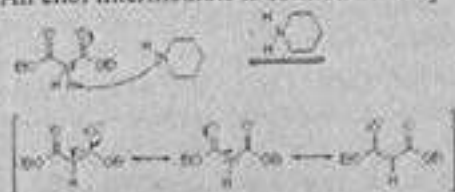


In this reaction the carbonyl group is an **aldehyde** or a **ketone**. The **catalyst** is usually a weakly **basic amine**. The active hydrogen component has the form<sup>9</sup>:

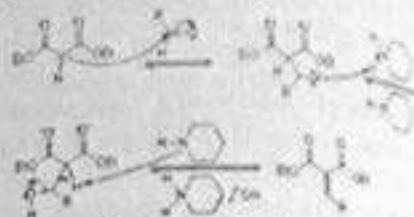
- **Z-CH<sub>2</sub>-Z** or **Z-CHR-Z** for instance **diethyl malonate**, **Meldrum's acid**, **ethyl acetoacetate** or **malonic acid**
- **Z-CHR<sub>1</sub>R<sub>2</sub>** for instance **nitromethane** where **Z** is an **electron withdrawing functional group**. **Z** must be powerful enough to facilitate hydrogen abstraction to the **enolate ion** even with a mild base. Using a strong base in this reaction would induce **self-condensation** of the aldehyde or ketone.

#### Mechanism of the Knoevenagel Condensation

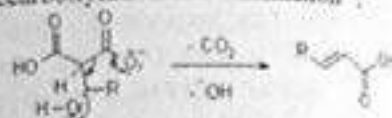
An enol intermediate is formed initially:



This enol reacts with the aldehyde, and the resulting aldol undergoes subsequent base-induced elimination.



The Doebner-Modification in refluxing pyridine effects **concentrated decarboxylation and elimination**<sup>10</sup>.



A reasonable variation of the mechanism, in which piperidine acts as **organocatalyst**, involves the corresponding **iminium intermediate** as the acceptor:

Thus in continuation of this work we have carried out the Knoevenagel type condensation reaction of phenanthrenequinone derivatives with 2-thioxo-4-oxazolidinone.

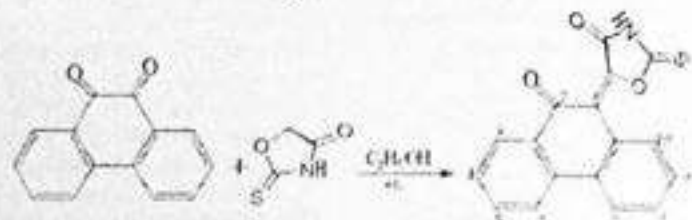
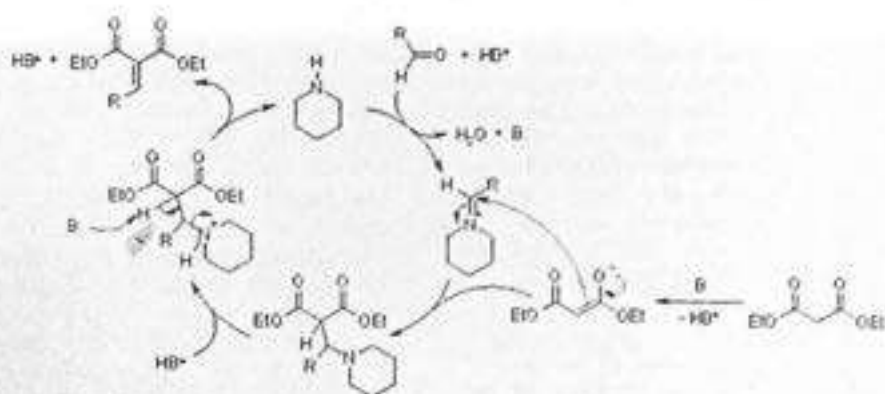
Phenanthraquinone is a tricyclic aromatic hydrocarbon (isomeric with anthracene) derived from coal tar, m.p. at 99 C, boils at 340 C, insoluble in water but is soluble in most organic solvents such as toluene, carbon tetrachloride, ether, chloroform, acetic acid and benzene. It is a white crystalline substance with a bluish fluorescence. It is used in the synthesis of dyes, explosives and drugs. It can be used as a feed stock of carbon black. We have explored the synthetic and mechanistic aspect of phenanthrenequinone condensation reaction with active methylene reagent 2-thioxo-4-oxazolidinone and investigate their configuration by semiempirical methods. The structural features of all the spiro and non spiro compounds have been



characterized by physicochemical techniques including IR and  $^1\text{H}$ NMR.

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Reaction of phenanthra enequinone with 2-thioxo-4-oxazolidinone

*[Signature]*  
Principal