

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,
Jaipur, Rajasthan
Principal
Kanoria PG Mahila Mahavidyalaya
JAIPUR

Sponsored by
Association of Chemistry Teachers;
Mumbai, Maharashtra
Department of Science & Technology
Jaipur, Rajasthan

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

Editors:

Dr. Kumud Tanwar

Department of Chemistry
Kanoria Mahila PG Mahavidyalaya,
J. L. N. Marg, Jaipur, Rajasthan

Dr. Atul K. Bhatnager

Department of Chemistry
B. B. D. Government College
Chimanpura (Shahpura), Jaipur

Dr. Ashok K. Kakodia

Department of Chemistry
S. G. G. Government College
Banswara, Rajasthan

Authors are responsible for the views, opinions expressed here and neither Editors nor Publishers are accountable in any manner.

Permission is needed for reproduction in any form.

Copyrights ©2017 by the Instrumentation Techniques for Research in Chemical Sciences.

Published by: Convener WITRCS – 2017, Kanoria PG Mahila Mahavidyalaya, Jaipur

ISBN: 978-93-5291-367-1.

Seans

Principal
Kanoria PG Mahila Mahavidyalaya
JAIPUR

	structural analysis (with spectral reference)	
	Sharma	57-60
24.	Alternative of Plastics: Biodegradable Starch-based Bioplastics. Rohi Verma, Kirti Srivastava, Pratibha Singh, R.S Jagadish	61-63
25.	Spectrophotometric studies of various Zn (II)-heterocyclic thiophosphate systems. Jasvinder Kaur	64-66
26.	Thermochemical characterization of clay by Thermogravimetric and Differential Thermal Analysis (In the special reference of Bikaner, Rajasthan's clay) Divya sharma	67-71
27.	Phytochemical and pharmacological potential of Saraca asoca (Ashoka): A Review. Sakshi Sharma and Reema Srivastava	72-74
28.	Comparative Analysis of Physicochemical Parameters of upstream site and downstream site of Haro River, Ghatol, Banswara, Rajasthan. Manish Kunwar Sisodiya, Lalit Choudhary, Pooja Joshi and Seema Bhardwaj	75-77
29.	Effects of Fluoride on Human Health in Rajasthan. Neha Goyal Dr. S. S. Dulawat	78-79
30.	Fluoride Levels in Ground Water Of Beawar City and Nearby Area A.K Siroya, Nisha Siroya, O.P Siroya	80-83
31.	Microwave Assisted Synthesis and Biological activity of [5(furan-2-yl)-phenyl]-4,5-carbothioamide -pyrazolines. Bhupendra K. Sharma, Ashok K. Kakodia, Praveen Meena, Ramesh K. Menaria	84-86
32.	Green Chemistry for Sustainable Development. Ritu Saharan	87-88
33.	Functionalized Graphene/Conducting Polymer Matrix as a Better Supercapacitor Material. Nidhi Agnihotri and Amitabha De	89-92
34.	Biosorption technique based on metal binding capacities for Wastewater treatment Sarita Singhal, Ritu K. Gupta and Rita Gupta	93-98
35.	Synthesis of Biologically Active Chalcones of Substituted Indole-3-Carbaldehyde under Ultrasonic Irradiation. Meenakshi Jain, Maya Agarwal, Madhuri Modi	99-100
36.	Toxicity of Transition metal complexes with Schiff base Ligands. Rekha Mithal	101-102
37.	A Review on phytochemistry and ethnomedicinal uses of some important Ipomoea species. Suneeta Rao, Taruna Sethi, M.P.Dobhai and M.C.Sharma	103-105
38.	Kinetics and Mechanism of Electron Transfer Reactions : Oxidation of Lactic Acid by Potassium Permanganate in Acid Perchlorate Medium Neeru Razdan	106-108
39.	Electro Chemistry: Applied in Decolourisation of Dye Effluents. Renu Bala and P.S.Verma	109-112
40.	Removal of Cu(II) from synthetic textile effluent using Tamarindusindica bark: A kinetic and thermodynamic study. Sudesh, Varsha Goyal, Arti Mishra	113-115
41.	An Efficient Approach to Synthesize Substituted Sulfonohydrazide Derivatives and their Characterization. Sunita Ghiya, Pratibha Payal, Y. C. Joshi	116-117
42.	Effect of water pH on Fish growth in the Haro Dam, Ghatol, Banswara (Raj.) Lalit Choudhary, Manish Kunwar Sisodiya and Seema Bhardwaj	

A one pot synthesis of fused heterocycles

Swati Singh¹ and Sunita Shekhawat²

¹Department of Chemistry, Kanoria PG Mahila Mahavidyalaya, Jaipur; ²Department of Zoology, Kanoria PG Mahila Mahavidyalaya, Jaipur

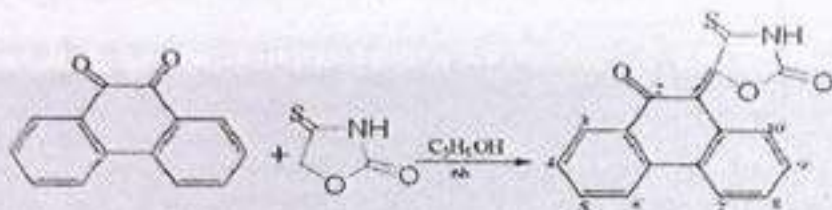
Abstract

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, α -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.

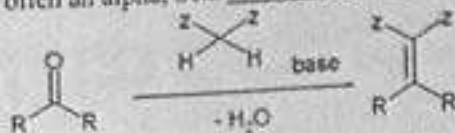
The increased interest in heterocyclic compounds is primarily due to high biological activity of some natural compounds of this group¹⁻³. Active methylene heterocycles incorporating toxophores such as and have been reported to possess a wide spectrum of therapeutic activities. Phenanthraquinone derivatives exhibit numerous pharmacological activities like

antioxidant⁴, antimalarial⁵, 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 tetracycline⁶.

The **Knoevenagel condensation** reaction is an **organic reaction** named after **Emil Knoevenagel** is a modification of the **Aldol condensation**^{7,8}.

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**.

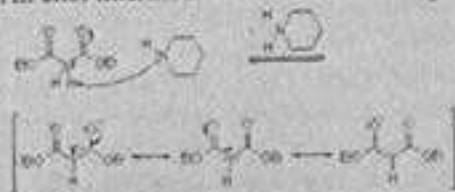


In this reaction the carbonyl group is an **aldehyde** or a **ketone**. The **catalyst** is usually a weakly **basic amine**. The active hydrogen component has the form⁹:

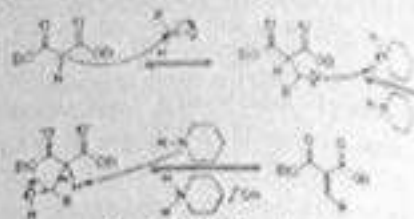
- **Z-CH₂-Z** or **Z-CHR-Z** for instance **diethyl malonate**, **Meldrum's acid**, **ethyl acetoacetate** or **malonic acid**
- **Z-CHR₁R₂** for instance **nitromethane** where **Z** is an **electron withdrawing functional group**. **Z** must be powerful enough to facilitate hydrogen abstraction to 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

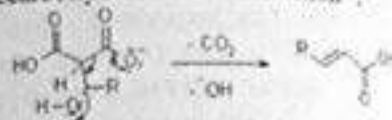
An enol intermediate is formed initially:



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**¹⁰.



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

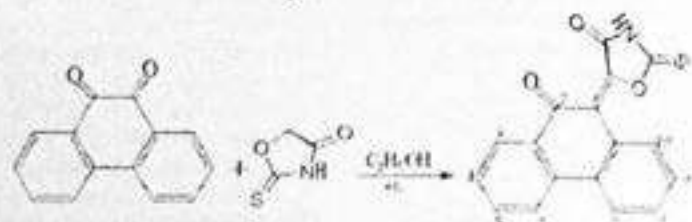
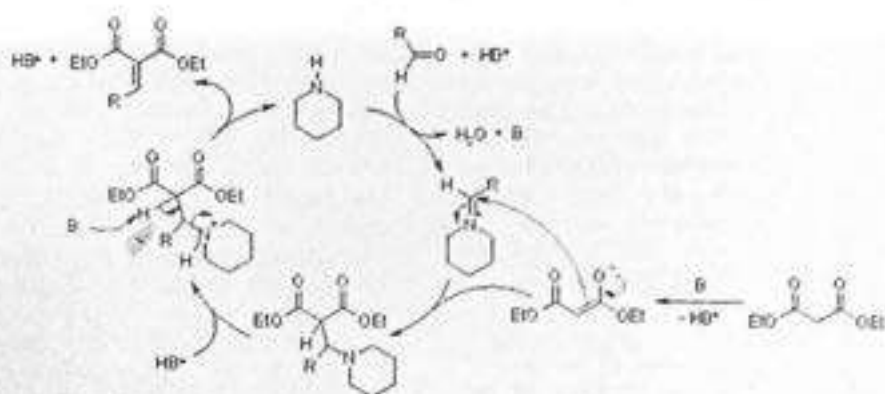
Thus in continuation of this work we have carried out the Knoevenagel type condensation reaction of phenanthrenequinone derivatives with 2-thioxo-4-oxazolidinone.

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 ^1H NMR.

REFERENCES:

1. Joshi K.C. and Chand P., *Pharmazie*, 1982, 37, 1.
2. Kornet M.J. and Thio A.P., *J. Monatsch. Chem.*, 1976, 19, 892.
3. Whiteside C.W. and Whitesitt C.A., *J. Med. Chem.*, 1974, 17, 1298.
4. Zhu YZ, Huang SH, Tan KH, Sun J, Whiteman M & Zhu Y C, *Nat Prod Rep*, 21, 2004, 478; (b) Ip S P, Yang H, Sun H D & Che C T, *planta Med.* 68 2002, 1077; (c) Cao E H, Liu X Q, Wang J J & Xu N F, *Free Radical Biol Med*, 20, 1996, 801.
5. Adam W, Kliem U, Mosandl T, Peters E-M, Peters K & Schnering H G V, *J Org Chem*, 53, 1998, 4986.
6. Katritzky A.R. and Pozharskii A.F., *Hand book of Heterocyclic Chem.*, Elsevier, 2000.
7. Edmondson S., Danishefsky S.J., Lorenzino L.S. and Rosen N., *J. Am. Chem. Soc.*, 1999, 121, 2147.
8. Jones, G. *Org. React.* 1967, 15.
9. Knoevenagel Emil. "Condensation von Malonsäure mit Aromatischen Aldehyden durch Ammoniak und Amine". *Berichte der deutschen chemischen Gesellschaft*, 1898, 31 (3), 2596-2619.
10. March, J., *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (3rd ed.), New York: Wiley, 1985, ISBN 0-471-85472-7.



Reaction of phenanthra-9,10-quinone with 2-thioxo-4-oxazolidinone