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Research Article

Synthesis and Characterization of Novel Benzoxazole Schiff Base Derivatives

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ABSTRACT

The synthetic work in this study was successfully carried out as planned, with all reactions yielding the expected compounds. A series of 2-(2-arginomethylene)hydrazyl)benzo[d]oxazole derivatives was synthesized using appropriate synthetic routes. The newly obtained compounds and intermediates were purified through recrystallization or column chromatography and further characterized using various physical and spectral techniques. Infrared (IR) spectroscopy showed characteristic peaks at 2795.34 cm^{-1}, 2908.97 cm^{-1}, 2713.33 cm^{-1}, 1660.90 cm^{-1}, and 1594.92 cm^{-1}. Proton NMR analysis displayed signals at δ 10.58 (NH), 8.55, 7.39, 8.78, 8.59, and 7.72 ppm. Mass spectral analysis confirmed the molecular ion peak at m/z 327, supporting the proposed molecular structure. Thin-layer chromatography (TLC), IR, ^{1}H-NMR, and mass spectra collectively confirmed the successful synthesis of benzoxazole Schiff base derivatives. Among the derivatives, the compound containing 2,4-dinitrobenzaldehyde exhibited particularly promising physical and spectral properties, suggesting its potential significance.

INTRODUCTION

1.1 Chemistry Of Benzoxazole

A heterocyclic compound or ring structure is a cyclic compound that has atoms of at least two different elements as member of its rings. Among all the heterocyclic compounds, benzoxazole[1] is one of the most important heterocyclic exhibiting remarkable pharmacological activities. Benzoxazoles is a organic compound, which has benzene fused with oxazole ring, oxazole[2] is 1,3-azole having oxygen atom and a pyridine type nitrogen atom at 3-position in a five membered ring.

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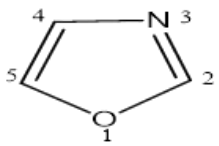
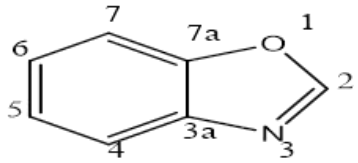




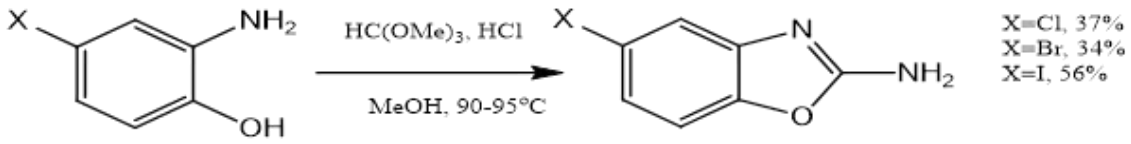
Benzoxazole is 1-oxa-3-aza-1H-indene, having molecular formula of C_7H_5NO, with melting point and boiling point of 29-30ºC and 182ºC.[3] Benzoxazole is a planar molecule with conjugated π electrons sectate in the cyclic system. The lone pair of electrons on nitrogen, which is co-planar with heterocyclic ring and therefore not involved in delocalization, confers weakly basic properties.

The electronegativity of the N- atom attracts electrons so that C-2 is partially electropositive and therefore susceptible to nucleophilic attack. However, electrophilic substitution of oxazoles takes place at the electron -rich position C-5 preferentially. More relevant to palladium chemistry, 2-halooxazoles or 2-halobenzoxazoles are prone to oxidative addition to pd(0). Even 2-chlorooxazole and 2- chlorobenzoxazole are viable substrates for the pd-catalyzed reactions.

1.2 Synthesis of halobenzoxazoles

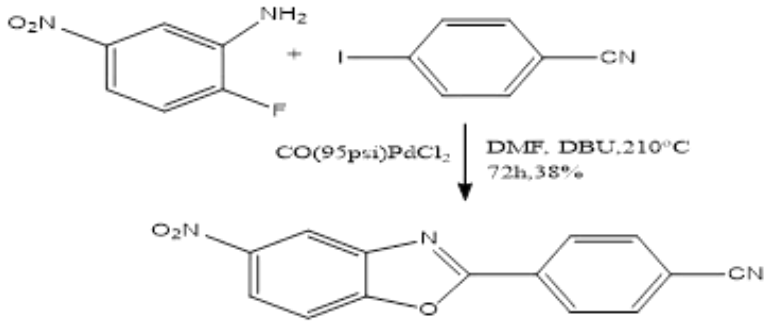
1.2.1. Sandmeyer reaction

While halogenation and Sandmeyer reaction are suitable for preparation of oxazolyl halides, benzoxazolyl halides with halogen on the benzene ring moiety may be synthesized via other approaches. For instance, 5-halobenzoxazoles[4] were prepared by treating 4-halo-2-aminophenols with trimethyl orthoformate and concentrated aqueous HCL.



1.2.2. Carbonylation

2-Aryl and 2-heteroaryl-bezoxazoles were prepared by Pd- catalyzed three-component condensation of aryl halides with o-aminophenols and carbonmonoxide followed by the dehydrative cyclisation[8,9]. A variant of such methodology using o-flourephenylamines in place of o-aminophenols was used to synthesized arylbenzoxazoles.

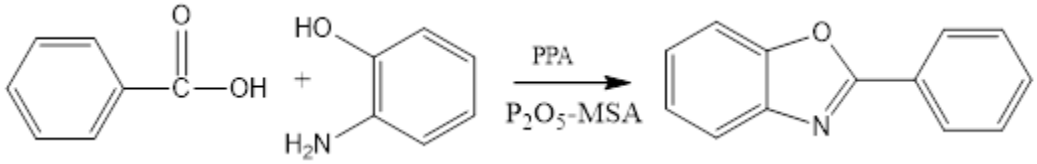


1.2.3 Other Reactions of benzoxazole

1.2.3.(A) Reaction with acids

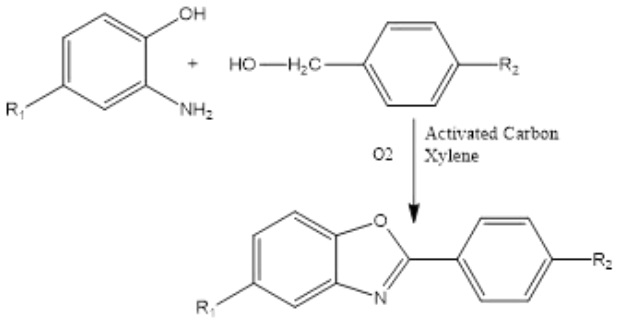
2-aminophenols can cyclize to benzoxazoles in the presence of carboxylic acids of upon heating to high temperature in the presence of a dehydrating

agent (polyphosphoric acid, phosphorous pentoxide- methanesulphonic acid , H3BO3)[5]. When equimolar amounts of 2-aminophenols and alkyl or arylcarboxylic acids are heated to temperature of 140-220°C are required for the formation of the corresponding 2-alkyl or 2-arylbenzoxazoles.



1.2.3.(B) Reaction with aldehydes

2-arylbenzoxazoles were directly synthesized from substituted 2-aminophenols and aldehydes in the presence of activated carbon in xylene under and oxygen atmosphere. A simple and efficient protocol as been developed for the synthesis of 2-arylbenzoxazole derivatives of potential pharmaceutical interest. The method involves reaction between 2-aminophenol and substituted aromatic aldehydes in the presence of anhydrous bismuth tricholoride as a catalyst in acetonitrile.



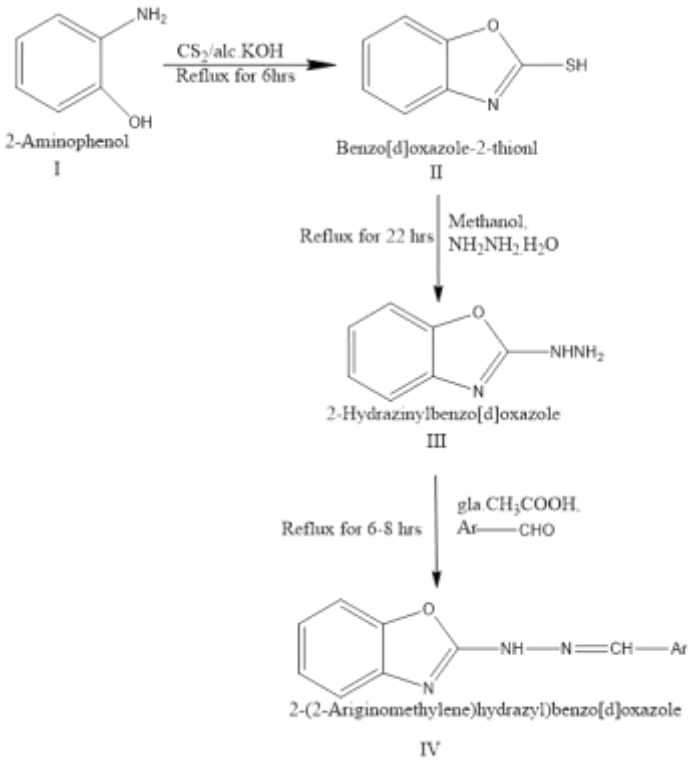
2. METHODOLOGY

SYNTHESIS

The scheme of synthesis for the designed benzoxazole derivatives was depicted below in scheme.

SCHEME:

2- (2-Ariginomethyelene) hydrazyl) benzo [d] oxazole IV



3. PROCEDURE

3.1 PREPARATION OF BENZO [D] OXAZOLE-2-THIOL

10.9g of 2-aminophenol,6.19ml of carbon disulphide, 5.65g of potassium hydroxide,15ml of water taken in a 250 ml RBF and refluxed in 100ml of 95% ethanol for 3-4 hours . Later charcoal was added continuously , refluxed for 10 minutes and filtered, the filtrate was heated up to 70-80^{0}C and 100ml warm water was added, 5% glacial acetic acid was added and stirred vigorously. The product was obtained as crystals and placed refrigerator for 3h for further crystallization. The product was filtered and dried. The dried product was recrystallized with ethanol.

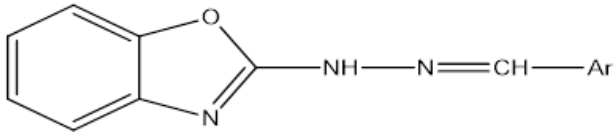
3.2 PREPARATION OF 2-HYDRAZINYLBENZO [d] OXAZOLE

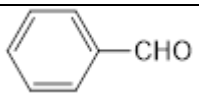
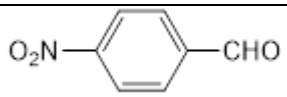
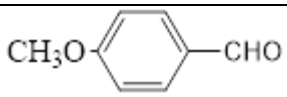
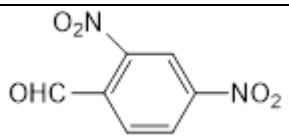
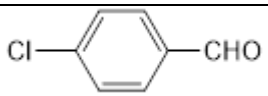
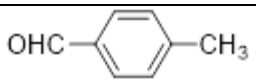
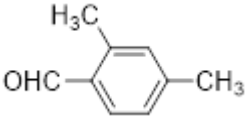
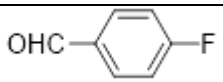
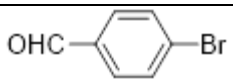
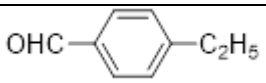
Equimolar quanities of benzo[d]oxazole and 99% hydrazine hydrate were dissolved in methanol and kept reflux for 20-22 hrs. The precipitate obtained was filtered washed with cold alcohol and dried.

3.3 GENERAL PREPARTION OF SCHIFF' BASE(IVA-E)

An appropriate aromatic aldehyde and 2-hydrazinylbenzo[d]oxazole(III) were dissolved in methanol , 1-2 drops glacial acetic acid was added and refluxed for 6-8h.The mixture was kept in refrigerator overnight. The product obtained was filtered, dried and purified by recrystallization.

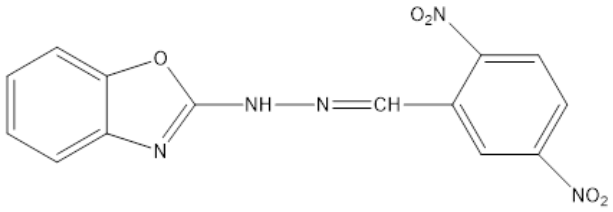
4. Physical data of 2-(2-Ariginomethyelene) hydrazyl) benzo[d]oxazole IV



Sr. No.	Compound	Ar	Molecular formula	Molecular weight	Melting point	Yield (%)
1	IV-a		$C_{14}H_{11}N_3O$	237.26	220	68
2	IV-b		$C_{14}H_{10}N_4O_3$	282.26	235	66
3	IV-c		$C_{15}H_{13}N_3O_2$	267.29	246	60
4	IV-d		$C_{14}H_9N_5O_5$	327.26	272	75
5	IV-e		$C_{14}H_{10}ClN_3O$	271.70	240	60
6	IV-f		$C_{15}H_{13}N_3O$	251.29	255	70
7	IV-g		$C_{16}H_{15}N_3O$	265.32	272	82
8	IV-i		$C_{14}H_{10}FN_3O$	255.25	256	66
9	IV-j		$C_{14}H_{10}BrN_3O$	316.16	260	78
10	IV-k		$C_{15}H_{15}N_3O$	265.32	275	75

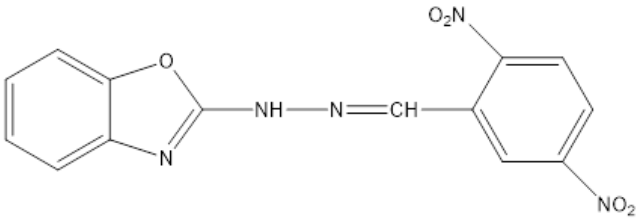
5. SPECTRAL DATA:

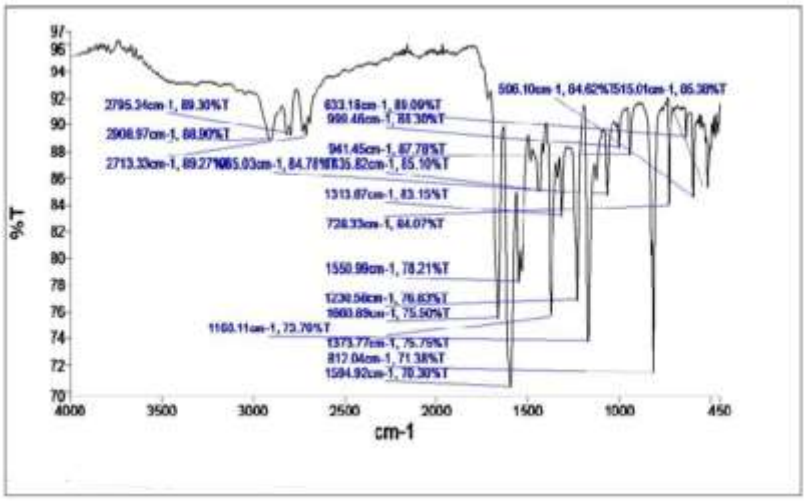
Spectral data of : 2-(2-Ariginomethyelene) hydrazyl) benzo[d]oxazole IV



- **Molecular formula:** $C_{14}H_9N_5O_5$
- **Mol .wt:** 327
- **IR (KBr) cm-**1:
  - CH-2795.34cm,CH-2908.97cm, CH-27
  - CH-1660.90cm,CH-1594.92cm
- **^{1}H NMR (300 MHz) (DMSO):**.
  - NH-10.58 CH-8.55
  - CH-7.39 CH-8.78
  - CH-8.59CH-7.72
- **Mass spectrum (ESI)** mass peak was observed at 327.

IR Spectral data of 2-(2-Ariginomethyelene) hydrazyl) benzo[d]oxazole IV

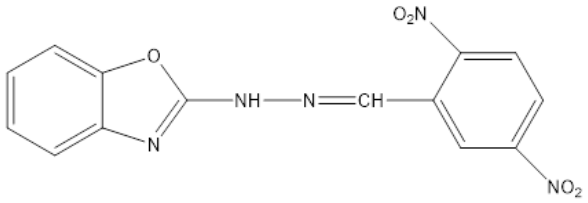


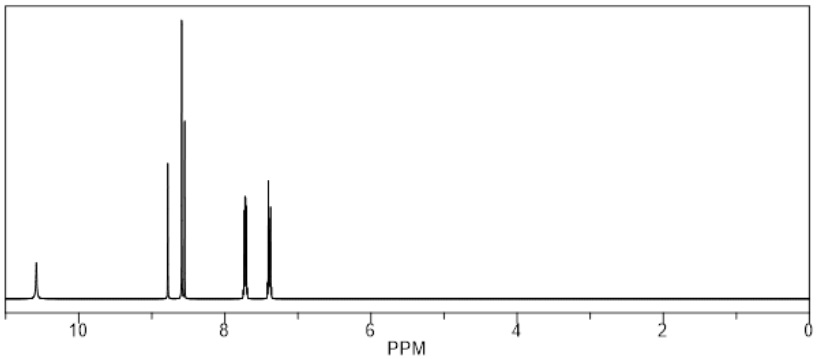


IR (KBr) cm^{-1}

- CH-2795.34cm,CH-2908.97cm, CH-27
- CH-1660.90cm,CH-1594.92cm

NMR Spectral data of 2-(2-Ariginomethyelene) hydrazyl) benzo[d]oxazole IV

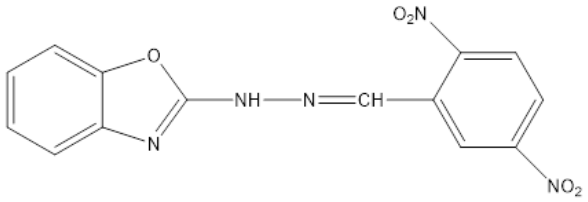


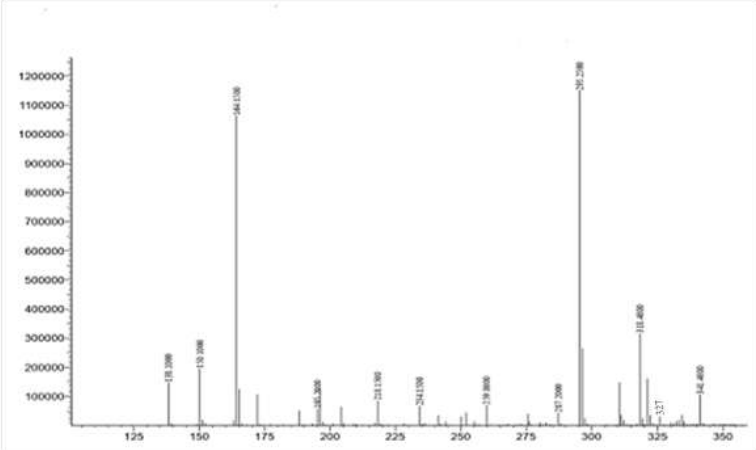


^{1}H NMR (300 MHz) (DMSO):.

- NH-10.58 CH-8.55
- CH-7.39 CH-8.78
- CH-8.59CH-7.72

Mass Spectral data of 2-(2-Ariginomethyelene) hydrazyl) benzo[d]oxazole IV





Mass spectrum (ESI) mass peak was observed at 327.

RESULTS AND DISCUSSION

1. Synthetic work of these studies has positively undergone as per the planning and as such in all the reactions carried, the expected compounds alone could be obtained.
2. The synthesis of 2-(2-ariginomethyelene)hydrazyl)benzo[d]oxazole derivatives by using appropriate synthetic routes.
3. Purified and characterized of all the new compounds, intermediates by recrystallization or by using column chromatographic techniques.
4. Characterized of newly synthesized compounds by physical and spectral method.

IR value

- CH-2795.34cm, CH-2908.97cm, CH-2713.33cm
- CH-1660.90cm, CH-1594.92cm

NMR value

- NH-10.58 CH-8.55
- CH-7.39 CH-8.78
- CH-8.59CH-7.72

Mass value molecular peak is obseverd at 327

CONLUSION

Newly synthesized compounds were characterized by TLC, IR, ^{1}H-NMR and Mass spectral analysis.

New benzoxazole schiff base derivatives was synthesised, all are showing good promising physical and spectral values. In this one derivarivative 2,4-dinitrobenzaldehyde showing more effective towards physical and spectral data.

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