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Investigations of $SnS_{0.5}Se_{0.5}$ ternary alloy crystals for their device application

Vibhutiba P. Jethwa^{a,*}, Kunjal Patel^b, V.M. Pathak^a

^a Department of Physics, Sardar Patel University, Vallabh Vidyanagar, 388120, Gujarat, India
^b Department of Physics, Government Science College, Vankal, Gujarat, India

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ABSTRACT

Alloy engineered single crystals demonstrates enhanced electrical and optoelectronic properties. For this purpose, Crystals of tin sulfoselenide $(SnS_{0.5}Se_{0.5})$ have been synthesized by the Direct Vapour Transport (DVT) technique. The elemental, morphological, structural properties and high crystallinity of DVT grown $SnS_{0.5}Se_{0.5}$ crystals were investigated by EDAX, SEM, XRD and HRTEM respectively. The core-level spectra of $SnS_{0.5}Se_{0.5}$ crystals were studied by X-ray photoelectron spectroscopy (XPS). The electrical properties of grown crystals were studied by Migh temperature electrical resistivity measurement and Hall effect measurement. The electrical resistivity measurement was studied in different directions in the temperature range of 297 K-673 K. The $SnS_{0.5}Se_{0.5}$ ternary alloy crystal exhibits anisotropic performance and showed higher conduction in the in-plane direction. The study of temperature-dependent vibrational properties was carried out by Raman measurement biasing voltages and intensities at an on/off period of 10 s and various photodetection parameters were also evaluated. The ternary alloyed crystal-based device exhibited good photoresponse and enhanced optoelectronic parameters.

1. Introduction

Layered metal chalcogenides have gained tremendous consideration because of their vital role in the improvement of future generation optoelectronic devices due to their strong light matter interaction [1,2]. Similarly, many metal chalcogenides have attracted attention because of their flexibility [3-6]. Among various metal chalcogenides tin sulfide and tin selenide exhibits excellent anisotropic behavior and are also recognized as good materials for photo-sensing as well as the photo conversion process. Moreover, they have been studied for their solar based applications as they have optimum bandgap and large absorption coefficient from UV to NIR light [7,8]. Such characteristics can make them a good candidate for thermoelectric applications and optoelectronic device applications [9-11]. The recent study on material characteristics suggests the excellent outcome in temperature-dependent electrical properties of tin chalcogenides (SnS and SnSe) so the researcher are focused on the thermoelectric, electronic and optoelectronic properties of group IV chalcogenides [12]. In addition to this tin chalcogenides are low toxic, earth abundant and low-cost materials. More interestingly, tin chalcogenides are extremely suitable as crystals,

nanocrystals, thin films and alloys with manageable appropriate morphology, size and composition for adjustable electronic properties [13,14]. As known, selenium doped tin sunfide can be an effective high performance optoelectronic device material [15]. It has been reported that with the doping of selenium in tin sulfide, the photoconductivity, carrier concentration and photoconversion efficiency increase [16]. The bandgap of ternary alloys could be perfectly tuned for a better optoelectronic device with doping of selenium [17]. It is confirmed that under the strategy of alloying mechanism, it is possible to improve the physical, chemical, optoelectronic and electronic properties of pristine SnS and SnSe [18]. Hereinafter there is surge of interest in Se doped SnS to have improved, cost effective and eco-friendly photosensitive application.

However, up to this time, most crystal based photosensitive devices have been constructed to be operated by an external power supply. So, there is a limitation in wireless environmental sensing applications. It can be overcome by fabricating self-powered photo sensing devices, which can work individually and wirelessly. This is a crucial research orientation for the next generation photo sensing device [19–21]. To the best of our knowledge, here we first time report the self-powered photo

* Corresponding author. *E-mail address:* jethwavibhuti95@gmail.com (V.P. Jethwa).

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Research Article







Structural, electrical, and optical properties of DVT-grown SnX (X = S, Se) crystals

Vibhutiba P. Jethwa^{1,*} (), Kunjal Patel², Anand Patel¹, and V. M. Pathak¹

¹ Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat 388120, India ² Department of Physics, Government Science College, Vankal, Surat, Gujarat, India

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ABSTRACT

Transition metal chalcogenides have become highly accessible nowadays for their outstanding sensing ability. Specifically, tin sulfide (SnS) and tin selenide (SnSe) are effective candidates for future electronic devices. Here, we synthesized P-type SnS and SnSe-layered crystals. The layered growth mechanism, high crystallanity, and phase transition of grown materials were confirmed by SEM, HR-TEM, and XRD, respectively. The X-ray diffractogram reveals the orthorhombic phase of grown SnX (X = S, Se). The formation of structure and binding energy were confirmed by X-ray photoelectron spectroscopy (XPS). The study of temperature-dependent vibrational mode is carried out for SnX (X = S, Se). The temperature-dependent resistivity measurement was performed. The hall effect measurement was performed at room temperature to calculate the carrier concentration, conductivity, and mobility. The optical properties of SnS and SnSe have been studied. This study estimates the suitability of the SnX (S, Se) crystals for the fabrication of optoelectronic devices.

1 Introduction

Recently, research on IV–VI groups of semiconductors has gained much attention due to their electrical properties and potential application in solar cells [1–5]. Among these semiconductors, tin chalcogenides are important due to their layer property and less toxicity compared to other similar materials [6–10]. In particular, tin chalcogenides are substantial materials for technological applications as a result of their huge absorption coefficients and narrow bandgaps [11, 12]. Tin chalcogenides exhibit applications

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in diverse fields such as thermoelectric devices, nearinfrared photodetectors, semiconductor sensors, anode for lithium-ion battery, memory switching devices, and photocatalyst [8]. The sulfide and selenide of group IV–VI form a fascinating family of layered chalcogenides [13]. It is also found that tin sulfide (SnS) and tin selenide (SnSe) is more suitable for the solar spectrum [14, 15]. Tin chalcogenides, such as tin sulfide and tin selenide, stand out among other semiconductors due to their flexibility, anisotropic behavior, and suitability for photo-sensing and photo conversion [16]. The orthorhombic SnS and SnSe are reviewed in between the two-

Address correspondence to E-mail: jethwavibhuti95@gmail.com

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High-performance self-biased photodetectors based on Bi-incorporated ReSe₂ ternary alloys

ABSTRACT

Hetal Patel^{a,*}, Kunjal Patel^b, K.D. Patel^{a,**}

^a Department of Physics, Sardar Patel University, Vallabh Vidyanagar, 388120, Gujarat, India
^b Department of Physics, Government Science College, Vankal, 394430, Gujarat, India

Transition Metal Dichalcogenides (TMDCs) have recently been the focus because of their unique physical properties. Bi-incorporated ReSe₂ (Bi: ReSe₂) is a new member of the TMDC family with a triclinic structure that is optically biaxial and strongly anisotropic. In this work, we reported the effect of Bi doping in layered ReSe₂ crystals synthesized by the Direct Vapour Transport (DVT) method and studied the structural and optoelectronic properties in detail. The layered surface of the single crystals, the stoichiometric proportion of elements and the triclinic structure and phase purity of the material has been observed using Scanning electron microscopy (SEM), Energy dispersive analysis of X-ray (EDAX) and X-ray diffraction (XRD) respectively. The shifting in vibrational Raman modes has been observed by Raman spectroscopy at room temperature. The dynamic I-t characteristics of Bi_xRe_{1-x}Se₂ (x = 0.1, 0.5) ternary alloy-based photodetectors were studied successively. The anisotropy in the dynamic I-t characteristics of transition metal chalcogenides was studied due to their layered structure. The device showed higher photoresponse for the perpendicular to c-axis configuration than for the parallel. Our results showed that the ternary alloys based single crystals have great potential for application in photosensitive devices.

1. Introduction

Photodetectors are sensors that convert photon energy from electromagnetic waves into electrical signals. Photodetectors are widely used in a variety of applications, including optical communication [1], photon sensing, energy applications, and optical waveguides [2]. Unlike other Transition Metal Dichalcogenides (TMDC) materials, ReSe₂ is one of the least familiar members with a 1.2–1.3 eV indirect bandgap [3]. Doping impurities into 2D TMDC materials were reported by some researchers [4,5]. Herein, we report for the first time in Bi incorporated to ReSe₂. Many essential features of Bi, such as an insulating interior but highly conductive surfaces, colossal positive magnetoresistance even at ambient temperature, and mobility much exceeding that of standard materials, remain controversial despite significant efforts [6–10]. Bi, as a bulk material in the periodic table, has separated itself from the other elements due to its modest effective carrier masses and unusually long carrier mean free path [11].

Bulk bismuth exhibits more exciting and compelling ideal properties

than its electronic structure in thin films to transition Bi from semimetal to semiconductor or insulator [12,13]. On the other hand, there is a group of new 2D layered materials with highly asymmetric plane crystal structures. Layered materials like black phosphorus and arsenic alloys, including the monochalcogenides of group IV elements like Ge and Sn material like Rhenium Diselenide (ReSe₂) and Rhenium Disulfide (ReS₂) [14] have unique optical, electrical, thermal and mechanical properties because of their anisotropic nature [15]. Photodetection properties in Nb-doped ReSe₂ have been reported [16]. We detailed a study on Bi-doped ReSe2 as a self-biased photodetector. The Results demonstrate that the properties of ReSe2 could be changed by doping Bi alloying, and the Bi-doped ReSe₂ maintains good optoelectronic properties. TMDCs material also can provide previously undiscovered tenability on the properties of electrical, optical, thermal, and piezoelectric devices. As a result, a wide range of opportunities for developing conceptually new semiconductor device applications is now available [17].

In this article, the authors have discussed the growth and characterization of Bi-incorporated ReSe₂ ternary alloy crystal and their novel

* Corresponding author.

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^{**} Corresponding author.

E-mail addresses: hetalppatel4496@gmail.com (H. Patel), kdptflspu@gmail.com (K.D. Patel).



Journal of Molecular Structure



Molecular dynamics of diclofenac potassium at 300.15 K temperature: Insights from broadband dielectric, thermal and MD simulation analysis



J.B. Karakthala^a, H.P. Vankar^b, V.A. Rana^{a,*}

^a Department of Physics, School of Sciences, Gujarat University, 380009 Ahmedabad, Gujarat, India ^b Department of Physics, Government Science College, 394430 Vankal, Gujarat, India

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ABSTRACT

Diclofenac potassium (DK) has been categorised as a class II drug by the biopharmaceutics classification system (BCS) based on its high permeability and low solubility. Solubility and stability of such a pharmaceutical medicine must be increased to make a good clinical candidate, which can be accomplished by understanding its molecular dynamics. In the current study, experimental and computational techniques are used to investigate the structural characteristics and the molecular interactions of DK at 300.15 K temperature. The thermal analysis of DK has been done by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Molecular dynamics of DK is investigated through broadband dielectric spectroscopy (BDS) and molecular dynamic (MD) simulation. Complex permittivity spectra of DK were obtained over two frequency ranges: i) low frequency (20 Hz $\leq f \leq 2$ MHz) and ii) high frequency (0.2 $\leq f \leq 20$ GHz). Relaxation mechanism in DK takes place in two ways; one is associated with the re-orientation of whole molecule, so-called primary (α) relaxation and other is originated from the small angle reorientation or group rotation of DK, so-called secondary (β , δ , γ) relaxation. Interactions between molecules/atoms/ions form different types of bonds in the DK molecules. Among them, interaction through H-bond is discussed in detail. Orientational dynamics revealed through DRS data is further confirmed by the MD simulation study.

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1. Introduction

Identification of molecular interactions can help to explain various drug performances including solubility, stability, dissolution, bioavailability etc. [1–3]. A comprehensive understanding of molecular dynamics of pharmaceuticals unfolds a new research topic for physicists, chemists, and material scientists working in the subject of pharmaceutical research. The diclofenac potassium (DK) is chemically designated as 2-[(2,6 dichlorophenyl) amino] benzene acetic acid mono potassium salt; and is commonly prescribed for pain management in several inflammatory diseases [4,5]. DK has a strong reactivity and excellent tolerability due to its unique structural characteristics. Their mutual interplay defines the drug structural stability and inhibition activity [6]. Intramolecular H-bond, which was validated during the X-ray investigation [7] is one of the fundamental characteristics defining the diclofenac structure. The study of DK's structural and inter/intra molecular interactions

* Corresponding author.

can be helpful in the development of various DK-containing pharmacological products that are tailored to specific needs, such as enhancing the efficacy, tolerability, and comfort of the medication for the patient [6,8]. Additionally, the literature suggests that the intramolecular H-bond in DK is used to modify the medication with, for example, transition metals [9], cyclodextrin [10], or PEG [11], to boost its water solubility and oral bioavailability [6]. Since H-bond is crucial for either the DK modification or the cyclooxygenase inhibition, it is necessary to gain insight into specific inter/intra molecular H-bond interaction, which has been accomplished in the current work using thermal, spectroscopic and computational investigations. To the best of our knowledge, the above investigations are studied for the first time for the DK in its pure form.

In of view of drug applications, thermal analysis are capable of revealing important properties like phase transitions [12], stability [13,14], shelf life predictions [15], moisture content determination [13,16], purity determination [17] etc. Thermal analysis tools, DSC and TGA, are used here to understand chemical processes taking place in material with temperature and time. It is also used to explore the thermal effects present in DK and to examine its pu-



E-mail addresses: jignakarakthala@gujaratuniversity.ac.in (J.B. Karakthala), varana@gujaratuniversity.ac.in (V.A. Rana).

"Design, synthesis, characterization and biological activity of acetophenone hetrocycle via novel mannich base MCR ."

Kumar G. Gamit¹ and Navin B. Patel²

¹Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007, Gujarat, India. ²Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007, Gujarat, India

ABSTRACT:

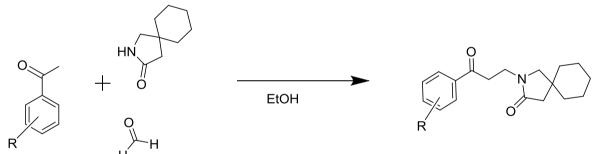
In this work ,Newly Fifteen-Compounds synthesized by Mannich base Multicomponent reaction .The synthesized compounds were characterized by using FT-IR, H^1 -NMR, C^{13} -NMR And Mass Spectrometry .The final compounds were evaluated for their Antibacterial activities using Agar-wel Diffusion method. The tested compounds show good to moderate activity with Inhibition zone value between 8 to 22 mm, when compared to reference Ampicilin and Ciprofloxacin. Among them compounds 4c and 4o show most promoting activity against E.coli, B.cereus and B.substilis.

KEYWORDS: Acetophenone, Antibacterial activity, gabapentin lacatam, Mannic base, Multicomponent reactions,.

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General Scheme:



R=3CH3,3CF3,3I,3NO2, 3OCH3,4OH,2OCH3,2OH, 2CH3,2CF3,2NO2,3H,3F,2OC2H5,2Br

I. INTRODUCTION :

The derivatives of C- Mannich base play an imperative role in a diverse fields, such as organic synthesis , medicinal chemistry, and agrochemistry.^[1] The Gabapentin lactam linked C-C mannich base scaffolds is widespread in a range of effective agrochemicals, and pharmaceuticals. For example, C-C products analog and derivatives have been exhibited to bear a array of pharmacological and biological properties such as Antibacterial,^[2] antifungal,^[3] Antitubercular, Anticancer,^[4] Antiinflammtory, antianalgesic, Anticonvulsant, antidepressant, anti-HIV, and Antidiabetic.^[5-7] Gabapentin lactam linked C-C mannich base has become a advantageous structure among the several types of organic compounds since the first isolation from natural indigo dye, . Because of the wide spectrum of functions in materials, pigments, pharmaceuticals, agrochemicals, and fragrances, Mannich product chemistry has fascinated extensive attentions from scientific society in the last few decades^{-[8]}

Multicomponent reactions (MCRs) are single-pot transformations utilizing more than two starting components, Gabapentin lactam are a unique class of Nitrogen and carbonyl containing heterocyclic compounds with vital Medicinal activities. This molecular diversity offers a spacious range of pharmacological properties.^[10] In consideration of auspicious properties of Acetophenone scaffolds Gabapentin lactam, and formaldehyde, the design and construction of new functionalized hybrid skeletons, which bearing all these three moieties may emerge as an crucial device in the organic synthesis.

N-containing heterocyclic compounds are attracting increases significance among the synthetic organic in the light of history owing of their abundance in various naturally occur product and the application in chemistry, material and biological science. ^[11-14]

Synthesis and in Vitro Biological Activity Study of Novel Phenol Mannich Base Analogs Containing Spiroheterocycle as Core Compound

Kumar G. Gamit and Navin B. Patel

ABSTRACT

The condensation reactions between Gabapentin lactam and phenols have been carried out in the presence of formaldehyde for the synthesis of various mannich base series. To confirm the formation of these series of newly prepared mannich bases thus synthesized, various characterization techniques have been used, such as, GC-MS, 1H-NMR, 13C-NMR and FT-IR. Further their antibacterial and antifungal activities against pathogenic bacteria have been evaluated. These compounds show promising activities against the pathogenic bacteria, hence are useful as antibacterial and antifungal active compounds.

Keywords: Antibacterial Activity, Antifungal Activity, Formaldehyde, Gabapentin, Lactam, Phenolic Mannich Bases.

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K. G. Gamit*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat, India (e-mail: kumargamit0106@gmail.com) **N. B. Patel** Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat, India

(e-mail: drnavinbpatel@gmail.com)

*Corresponding Author

I. INTRODUCTION

The mannich base formation by the condensation reaction between the aldehyde, active hydrogen compounds, and amine, leading to produce Mannich bases. There are four different types of classification of Mannich bases, which includes c-type, S-type, N-type, and P-type mannich bases. Mannich bases are getting industrial importance due to their vast applicability in the various industrial synthesis processes, such as in paints, cosmetics, synthetic polymer products, water treatment chemicals, petroleum additives, paper and leather industries and in textiles industries [1]. Besides these, the most important application of the Mannich base is in the field of medicinal chemistry, it can be used to improve the solubility and distribution of the drug molecules into the human body. The hydrophobic properties of the drugs could be increased by inserting the polar group into the drug molecules through the Mannich base reaction. In addition to that, the lipophilic properties of the drug molecules could be enhanced, if the suitable amine containing reagent is utilized in the Mannich base reaction [2]. The phenolic Mannich bases are classified as the C-Mannich bases which tends to forms C-C bonds and are considered as a very important class of the compounds due to their biological activities such as antibacterial activities [3],[4], antimycobacterial activities [5],[6], anticancer and cytotoxic activities [7]-[9], anti-inflammatory activities [10],[11], antihepatitis-B activities [12,13], antiviral activities [14]-[16], and antifungal activities [17],[18], analgesic activities [19], anticonvulsant activities [20], [21], enzyme inhibition activities [22], antioxidant properties [23],[24], blood pressure regulation [25],[26], and platelet aggregation inhibition activities [27].

Gabapentin lactam is one of the gabapentin derivatives and it is considered to be useful as the neuroprotective agent in the retinal ischemia. It is also considered as the spiro compound as it contains two rings connected with single carbon atom, such spiro compounds are of great interest in the field of medicinal chemistry, the spiro carbon available in the structure gives the adjustment along the precise vectors and allows structure rigidity because of the unique conformational properties and complexity in the structure [28]-[32].

According to the growing demand and in a continuation of our work in the field of synthesis of chemically useful and pharmacologically active compounds, it seems to be of great idea to synthesize various heterocyclic spiro compounds having gabapentin lactam moieties as a core compound and evaluate their biological activities. This research work comprising the synthesis methodology of the novel spiroheterocyclic compounds containing the gabapentin lactam as a backbone of the compound, through the reactions between various derivatives of phenols, formal dehydes and gabapentin lactam.

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An efficient construction of quinoline-based hybrid scaffolds through palladium-catalyzed C—S coupling

Bhavik S. Makwana^a, Mayur I. Morja^b, Kishor H. Chikhalia^{a,*}

^a Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat, India
^b Department of Chemistry, Government Science College, Vankal, Surat-394430, Gujarat, India

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ABSTRACT

Organosulfides have prodigious value and significance in synthetic and biological chemistry. In this context, an efficient and operationally simple construction of quinoline based hybrid scaffolds has been achieved through palladium-catalyzed C—S coupling synthetic strategy. This strategy employs the reaction of 2-(2-chloroquinolin-3-yl)-3-phenylthiazolidin-4-ones with thiophenols under palladium catalysis. Some notable features of this methodology like high efficiency, good functional group tolerance and easily obtainable substrates provides a promising platform. The employed strategy is anticipated to be further utilized in developing direct transformations of inert haloquinoline into synthesis of medicinally important building blocks.

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Introduction

Over the last few decades, guinoline derivatives have attracted substantial interest among the medicinal chemistry community because of their promising physiological and chemotherapeutic properties [1]. Quinolines are key structural motif and ubiquitous in N-heteroarenes which have been usually found in many commercially available pharmaceutical products [2]. Camptothecin and some of its analogues are well acknowledged as clinically validated anticancer drugs [3]. In 2010, Rahul Jain and co-workers examined the role of quinoline and other comparable heterocycles which has resemblance of the quinoline nucleus used in the treatment of malaria [4]. Later on, Keri and Patil highlighted the potential of synthetically adaptable quinoline derivatives used against tuberculosis [5]. Based on various medicinal applications, it has been established to design outstanding structure endowed with quinoline nucleus. Furthermore, a vast variety of quinoline derivatives have been discovered to be useful in agrochemistry as pesticides, herbicides, and fungicides etc. [6].

4-Thiazolidinones have recently been emerged as key pharmacophores and play a vital role as therapeutic agents with a wide diversity of biological properties, such as anti-fungal, anti-bacterial, anti-tubercular, anti-inflammatory, anti-HIV, anti-diabetic,

* Corresponding author.

https://doi.org/10.1016/j.tetlet.2023.154462 0040-4039/© 2023 Published by Elsevier Ltd. anti-cancer, anti-epamastigote and antiarrhythmic [7]. The synthesis and biological activity of 4-thiazolidinone analogues have received a great deal of attention. Several derivatives of 4-thiazolidinone have been discovered to be selective bacterial enzyme inhibitors like Mur B, MptpB, HER-2 kinase, COX-1 and COX-2, HIV-RT etc [8]. Some exemplary biologically active compounds having both quinoline and 4-thiazolidinone nucleus are shown in Fig. 1 [9].

On the other hand, sulfur-containing organic compounds are a significant class of compounds that can be found in a wide range of natural products, bioactive substances, dyes, drugs, agrochemicals and functional materials [10]. Hybridizations of two or more different bioactive pharmacophores in a single molecule appears to exhibit better activity. [11]. To the best of our knowledge, scientists have concentrated more to the incorporation of quinoline coupled with 4-thiazolidinone and thiophenol in anticipation of enhancement of pharmacological characteristics. Hence, a hybrid quinoline, 4-thiazolidinone and thiophenol unit combination may contain promising biological features. Our ongoing attempts on development of bioactive compounds aims to molecular combination quinoline, 4-thiazolidinone, and thiophenol units in a single molecular framework.

Transition metal catalysed C-X (X = heteroatom such as O, N, or S) and C—C bond formation via cross dehydrohalogenative coupling (CDC) reaction has been emerged as an advantageous synthetic strategy in modern organic chemistry. It aims to rationalize the designing plethora of potent molecules in fewer

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E-mail addresses: chikhalia_kh@yahoo.com, khchikhalia@vnsgu.ac.in (K.H. Chikhalia).

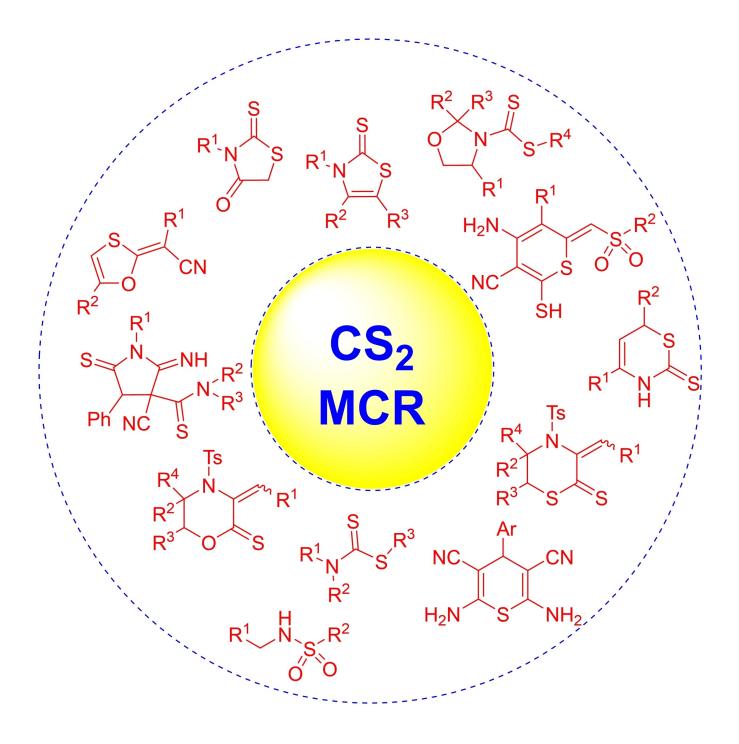




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Multicomponent Approaches Involving Carbon Disulfide

Mayur I. Morja,^[a] Riddhi H. Viradiya,^[b] and Kishor H. Chikhalia^{*[b]}



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Abstract: In present scenario, innovative carbon disulfideness, the use of easily obtainable starting compounds, and involving multicomponent protocols are extremely advantageous for practical and efficient construction of acyclic as well as heterocyclic building blocks. Carbon disulfide is well recognized synthetic component and has achieved the desirability of scientific community for the preparation of a variety of highly functionalized organic scaffolds. Carbon disulfide involving MCRs mostly advantage from other features such as bond-forming efficiency, resource effective-

atom-economy, which make these protocols useful environmentally benign alternatives, in care with the greener way in which organic chemistry is going on. In this review article, we have discussed the noteworthy topical advances in the promising region of carbon disulfide-involving multicomponent reactions. It highlight the prospects and confronts, emphasizing the diverse approaches established previously.

1. Introduction

The advancement in novel synthetic approaches for the straightforward generation of nitrogen, oxygen and sulfur containing-heterocyclic candidates have been prospered in recent decades. Their ubiquity in pharmaceuticals and several naturally occurring products demonstrate an extensive array of biological properties.^[1-4] Particularly, sulfur-containing heterocyclic moieties are the most principal types of pharmaceutically active chemical compounds, which are extraordinarily well founded among many biologically powerful synthetic substances, drugs, and so forth.^[5-7] Thus, S-bearing organic molecules have been broadly utilised in drug design and medicinal chemistry due to their pervasive combining capability.^[8] For instance, S-bearing compounds are present in more than onefifth of the highest 200 utmost-prescribed medicines. Sulfur is an imperative element in a diversity of biomolecules and proteins, for example chondroitin sulfate, heparin, and thiamine.^[9-10] Furthermore, sulfur-containing compounds are rational in many areas, such as organic, materials, and biological chemistry.^[11-14] Scientific studies have revealed that S-containing drugs can be utilised for the remedy of AIDS, cancer, anxiety and depression, Parkinson's disease, Alzheimer's disease, and other diseases.^[15-20] The S-containing heterocycles also play important role in the arena of photoelectric material owed to higher resonance energy linked with sulfur atom than another heteroatom.^[21-22] Thus, the expeditious construction of structurally diverse and complex S-containing (hetero)cyclic scaffolds is a significant pursuit in organic synthesis.

The multicomponent coupling reaction (MCR) is emerged as a prevailing synthetic devise to combine three or more organic components in a one-step operation to produce comparatively multifaceted molecular structures with high step- and atom economy.^[23–25] In 1850, Strecker reported a protocol for α -amino acid synthesis via three-component reaction comprising hydrogen cyanide, aldehydes and ammonia. This is formally the very pioneered MCR in the history of chemical science.[26-29] The capability to quickly construct structural complexity has been momentously enhanced by the expansion of MCRs with an extensive array of succeeding post-transformation tactics such as, intra or intermolecular SN₂, SNAr, metal-catalyzed crosscoupling reactions, deprotection-activation-cyclizations, cycloadditions, acid-base facilitated annulations, deprotection-cyclization, RCM (ring-closing metathesis), and radical cyclization, etc.^[30-31] On the other hand, carbon disulfide (CS₂) is one of the distinctive chemical synthons owing to their inclusive accessibility from several sources in low-price and stability which creates the essential role of CS₂ in organic chemistry. As ultimate building blocks of organic transformations, techniques that permit the selective involvement of CS₂ in MCR is well discovered and has gained substantial consideration from synthetic community. In this context, to assemble structurally complicated architectures starting from abundant and simple building blocks, MCR has viewed as an influential tool. The enlargement of chemical space through cooperative merging of CS₂ as coupling synthon and MCR offers unparalleled opportunities to synthesize diverse molecular frameworks with decisive applications in functional materials, drug discovery, and medicinal chemistry research. As a subject of fact, an extensive series of literature documents are now existing on CS₂-involving MCR; nevertheless, to the best of our knowledge no recent review available for the same area.

A large number of exertions have been made from numerous research teams across the world. This review is devoted to discuss and showcase topical advancement in the arena of CS₂-involving MCR systems, with a prominence on the reactivity, limitations, catalysis, substrate preparation and scope, as well as the mechanisms of these transformations. Particularly, the CS2-involving MCRs including the formation of five-membered heterocycles (2-thioxo-1,3-thiazolidin-4-one, 1,3-thiazole-2-thione, pyrrolidine, oxazolidine, 1,3-oxathiole), six-membered heterocycles (1,3-thiazine-2-thione, 1,3-benzothiazine-2-thiones, 1,4-thiomorpholine, 1,4-oxathiane-3-thiones, Thiopyran), and acyclic dithiocarbamate are delineated chronologically together with comprehensive mechanistic discussions.

[[]a] Dr. M. I. Moria Department of Chemistry, Government Science College, Vankal, Surat -394430, Gujarat (India)

[[]b] R. H. Viradiya, Prof. K. H. Chikhalia Department of Chemistry, Veer Narmad South Gujarat University, Surat -395007, Guiarat (India) E-mail: chikhalia_kh@yahoo.com



Facile synthesis of chromeno fused imidazolidinone derivatives via copper-catalyzed tandem O-arylation/oxidative acylation protocol

Prakashsingh M. Chauhan,^[a] Mayur I. Morja,^[b] Bhavik S. Makwana,^[a] and Kishor H. Chikhalia^{*[a]}

An efficient copper-catalyzed tandem reaction of 1,3-dibenzylimidazolidine-2,4-diones with ortho halo-benzaldehyde compounds toward chromeno fused imidazolidinone has been developed. This protocol proceeds via one-pot sequential intramolecular O-arylation (C–O bond formation) and oxidative acylation (C–C bond formation). The synthetic method has the advantages of easily available starting materials, good functional tolerance, and wide substrate scope, which make this protocol more sustainable and practical. Experimental outcomes demonstrate that radical pathway might be involved in these transformations.

Introduction

Heterocyclic compounds are ubiquitously embedded in several functional molecules. It plays a significant role in the design and discovery of novel pharmacologically active compounds.^[1] Among various heterocycles, chromone is one of the most important structural motifs which display a wide range of interesting biological activities such as antibacterial, β hydroxylase inhibitor (antagonist), antioxantihypertensive, idant, anti-inflammatory and antitubercular.^[2] Likewise, fused imidazolidinone and its analogues are omnipresent structural motifs, which exist in diverse pharmaceutical product. They found to possess a remarkable biological and pharmacological activities, such as anti-psychotic, anti-viral, and anti-inflammatory etc..^[3] Some of the representative bioactive molecules having chromone and imidazolidinone nucleus are demonstrated in Figure 1. Because of the significance of these two scaffolds, new approaches towards the synthesis of hybrid entity containing both chromone and imidazolidinone remains of high interest, which may benefit and stimulate the research arenas of drug discovery and chemical science. In view of these possibilities, we were tempted to develop a novel heterocyclic building block which incorporates both these units in the single molecular framework.

Nowadays, transition metal-catalyzed C–H functionalization reactions are becoming one of the most essential and influential tools for organic chemists to create carbon-

[a]	Dr. P. M. Chauhan, B. S. Makwana, Prof. K. H. Chikhalia
	Department of chemistry, Veer Narmad South Gujarat University, Surat,
	395007, Gujarat, India
	Tel: +91 9427155529
	E-mail: khchikhalia@vnsgu.ac.in

- [b] Dr. M. I. Morja Department of Chemistry, Government Science College, Vankal, Surat, 394430, Gujarat, India
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carbon and carbon-heteroatom bond.^[4] Particularly, direct cross dehydrogenative couplings (CDC) between two different C–H cores are emerged as the most important approach for the construction of C–C bonds. The CDC methodologies are extremely valuable owing to the minimization of waste and the costs associated with the prefunctionalization of starting materials.^[5] In context to the environmentally benign nature of the CDC approaches, numerous efforts have been in the development of synthetically and pharmaceutically important cyclic ketones through direct acylation of (hetero) arenes with aldehydes.

It is concluded from the literature survey that intermolecular CDC reaction of (aryl)aldehyde C-H bonds with olefin or arene C-H bond, as well as acylation of sp² C-H bonds using aldehydes, arose interest in the synthesis of aryl cyclic ketones.^[6-7] Various intramolecular CDC processes provides an insight to privileged bicyclic and tricyclic compounds with ketone functionality. For instance, some elegant and efficient protocol towards cyclic ketone formation include xanthone formation from 2-aryloxybenzaldehydes via cross-dehydrogenative coupling,^[8] formation of thioxanthones from 4-(3-methoxy-phenylthio)-2,2-dimethyl-2(H)chromene-3-carbaldehyde via ruthenium catalysis,^[9] synthesis of pyrazole-chromone through ionic liquid promoted annulation strategy and copper-catalyzed tandem protocol,^[10] intramolecular C–H cyclization of formyl-Narylformamides leading to indoline-2,3-diones isatins,^[11] synthesis of fluorenone,^[12] and synthesis of acridones via intramolecular dehydrogenative cyclization reaction.^[13] (Figure 2) However, these types of intramolecular transformations always require precursor which are needs to be prefunctionalized. Wu's group presented the palladium catalyzed tandem reaction of imidazo pyridines with 2chlorobenzaldehydes,^[14] but in this transformation use of the costly pd catalyst was mandatory (Figure 3). Therefore, further exploration of innovative and efficient methods under mild reaction conditions for the construction of chromenone fused heterocycles in an intermolecular fashion



Cu-catalyzed dehydrogenative C–O arylation for the synthesis of 6-methyl benzofuro[3,2-c] quinoline derivatives

Bhavik S. Makwana¹ Kishor H. Chikhalia¹

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Mayur I. Morja² | Prakashsingh M. Chauhan¹

IETEROCYCLIC

¹Department of Chemistry, Veer Narmad South Gujarat University, Surat, India ²Department of Chemistry, Government Science College, Vankal, Surat, India

Correspondence

Kishor H. Chikhalia, Department of Chemistry, Veer Narmad South Gujarat University, Surat 395007, Gujarat, India. Email: chikhalia_kh@yahoo.com

Abstract

A novel strategy for the synthesis of 6-methyl benzofuro [3,2-c] quinoline derivatives via copper-catalyzed dehydrogenative C-O arylation has been presented. Optimization studies have been carried out by varying various catalysts, bases, solvents, and other physical parameters. Keeping use of this dehydrogenative cross-coupling C-O arylation reaction, a variety of bioactive building blocks like fused benzofuro quinoline heterocycles were smoothly assembled in moderate to higher yields.

1 INTRODUCTION

Nitrogen, oxygen, and sulfur containing heterocyclic scaffolds are abundant in pharmacologically active substances [1]. Among them, quinoline heterocycles are the 22nd most prevalent ring system in drugs [2]. It is one of the heterocyclic structures that are among the most ubiquitous, found in both natural and synthetic compounds that possess significant biological or functional material characteristics [3]. Quinoline-fused structures that contain heterocyclic rings at different places are indeed more important. This structural motif is associated with certain biological activities such as antimicrobial, antimalarial, anticancer, anti-HIV, and antituberculosis [4]. Due to their significant biological functions, furan/benzofuran fused quinolines have gained a lot of interest in synthetic medicinal chemistry. As illustrated in (Figure 1) compound A has been investigated to be a neuroprotective agent and compound B is found to inhibit bone resorption and stimulate bone formation. Compound C (CCK2) and compound D (CCK3) are respectively used as an antitumor agent. Compound E has also been reported as a potential topoisomerase-II inhibitor [5]. Considering the various biological functions of these compounds, the design and synthesis of the new heterocyclic compounds containing benzofuro [3,2-c] quinoline structure would be beneficial to biological research.

Benzofuro[3,2-c] quinoline derivatives have been synthesized through various synthetic methods. Some of the reported pathways to construct this scaffold are demethyl-cyclization of 3-(o-methoxy phenvl)-1.-4-dihydro quinoline-4-ones [6], palladium-catalyzed C—H bond oxidative carbonylation reaction [7], a tandem azide intramolecular annulation and oxidation reactions of biaryl methyl azide precursors [8], microwave-assisted direct o-arylation of quinolones without metal and ligand condition [9], one-pot palladium-catalyzed synthesis via oxidative cyclization of arylols and iodoarenes [10], phosphine free palladium-catalyzed direct arylation of 4-phenoxy quinolines in the air [11], one-pot C—H functionalization/ cross-coupling reactions using quinoline as a substrate and ligand through N-Pd interaction [12], via a sequential chlorination/demethylation intramolecular cyclization pathway [13], and Pd-catalyzed substrate or solvent-controlled regioselective arylation of quinolin-4 (1H)-ones using diaryliodonium salts [14] (Figure 2). These methods are either multistep reactions or performed using expensive metal catalysts like palladium. As a result, the search for alternative methodologies, which provide a clear and shortest approach to designing these frameworks is of prime significance. In this context, transition metal-catalyzed intramolecular arylation, which includes C-H activation as a vital step emerged as a strong and adaptable method for synthesizing several

Tetrahedron

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Transition metal-free synthesis and functionalization of phenothiazines

<mark>Mayur I. Morja</mark>^{a,**}, Kishor H. Chikhalia^{b,*}

^a Department of Chemistry, Government Science College, Vankal, Surat, 394430, Gujarat, India
^b Department of Chemistry, Veer Narmad South Gujarat University, Surat, 395007, Gujarat, India

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ABSTRACT

Phenothiazines are prominent as a remarkable class of heterocycles having multifaceted uses in material science as well as medicinal chemistry. Their practical, facile and easy preparation remains an incessant challenge. Diverse tactics have been developed in this intention for a long time. Synthesis of phenothiazines in the absence of transition metal has received a lot of attention because of its added benefit. However, none of previous reviews has been explicitly dedicated to discuss and summarize the outcomes accomplished in rapidly rising field of the transition metal-free synthesis and functionalization of phenothiazines. In this review article, we have emphasized the use of electrocatalysis, organo-catalysis, micelles (SDS) catalysis, acid catalysis, base catalysis, iodinecatalysis, nitrosonium ion catalysis, and photocatalysis in the construction and functionalization of phenothiazines. Various reaction parameters such as the use of commercially available reagents, easily accessible starting materials, and ease of preparation (high yields, short reaction times, reasonable temperatures, limited byproducts) are covered in the discussion along with the scope of reaction and limitations.

1. Introduction

Phenothiazines (PTH) signify a class of sulfur- and nitrogen-based heterocyclic compounds with extensive application in the manufacture of pigments and dyes since the early period [1]. Research related to properties and new synthetic methods of such heterocyclic compounds seems to be stimulating for both industrial applications and fundamental research. The exploitation of innovative synthetic approaches for the straightforward construction of phenothiazine scaffolds has prospered in recent years because of their omnipresence in numerous biologically active molecules and pharmaceuticals. Synthetic phenothiazines (with piperidine, piperazine-ethanol, piperazine-ethyl, methylpiperazine, or aliphatic side-chain) and/or phenothiazine-derived agents e.g., cyproheptadine, dimetothiazine, imonostilbenes, thioxanthenes, benzepines, and tricyclic antidepressants have been effective in the therapeutics of a number of medical situations with broadly different cytology. Emphasizing the superiority of the phenothiazine chemical assembly as a core molecular template to interact with an extensive range of biological courses, phenothiazine-derived agents and/or synthetic phenothiazines revealed their practicality in the treatment of manifold medical conditions with broadly different symptomatology and etiology. These butterfly shaped molecules display remarkable and diverse

pharmacological activities, and hence establish the central unit for many important drugs [2]. For the dealing of psychotic diseases, more than 100 phenothiazine derivatives such as Chlorpromazine have been exploited till the date. In the drug discovery field, phenothiazine derivatives are well recognized for their antioxidant potential, anticancer activity, antitubercular activity, histamine H1 antagonist, cholinesterase inhibitor, and several other biological activities [3]. Fig. 1 exemplifies the illustrative examples of phenothiazine-bearing bioactive molecules.

Nevertheless, their significance is not restricted to medicinal purposes only. In addition, the electroactive, extensive π -conjugation, and rigid skeletons distinctively demonstrate intense luminescence and high molar absorption coefficients to favour utilization prospective in optoelectronics [4]. The ionization potential of 6.73 eV and the existence of electron-rich nitrogen and sulfur heteroatoms is well applicable for building the D-A materials with improved ICT features [5]. 10H-Pheno-thiazine has a powerful electron donor nature than other amines, even better than iminodibenzyl, carbazole, tetrahydroquinoline, triphenyl-amine, and many other N-heterocycles [6]. Now, the development of readily accessible and inexpensive organophoto catalysts as the alternatives of metal-cored PCs has engrossed general consideration [7]. From a synthetic point of view, N–H bonds of phenothiazines have low dissociation energy. Thus, it could produce stable persistent N-centered

* Corresponding author. ** Corresponding author.

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E-mail addresses: mayurbhai.morja@gujgov.edu.in (M.I. Morja), chikhalia_kh@yahoo.com (K.H. Chikhalia).



Evaluation of Growth and Reproductive Parameters of Tomato Plant (Solanum Lycopersicum L.) For Application of Organic and Inorganic Fertilizers

Ms. Arpana A Rathod, Dr. Meghna R Adhvaryu

Department of Botany, Government Science College, Vankal, Ta. Mangrol, Dist. Surat - 394430, Gujarat, India

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ABSTRACT

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Page Number 227-232 Reproductive biology provides information on life forms like rate of flowering, type of breeding system, plant-pollinators interaction, fruit and seed output, overall fitness and survival of the species. Present work has been focused to determine the effects of synthetic and organic fertilizers application on the growth parameters like stage of plant development, plant height, number of leaves, number of flowers, flowers to fruits conversion and %yield. Field experiments were conducted in the farms located in Jahangirabad area of Surat city from 2017 to 2018. Season for experiments was chosen between month of October to April where average low temperature of Surat ranges between 15°C-21°C and average high temperature ranges between 25°C-35°C. The treatments consisted of two different fertilizers namely synthetic inorganic fertilizer (SFT) consisting of NPK and organic fertilizer (OFT) chiefly consisting of cow-dung/buffalodung/poultry manure. Three plot of 30 x 02 sq. ft area was selected to grow 30 plants of Tomato. One plot was designated as Control group where no pre-treatment (CT group), one plot treated with SFT group and the other with OFT group. Results suggest that OFT treated plant showed increased plant height, quantity of leaves (per branch & plant) and its weight (fresh & dry), quantity of flowers and fruits, diameter and length of fruit, quantity and weight of seed per fruit, nutrition of fruit as compared to Control group and well comparable with SFT treatment. Thus, it is concluded that use of organic fertilizer is equally beneficial as compared to the inorganic fertilizer.

Keyword: Reproductive, Fertilizer, Organic, Inorganic, Tomato

I. INTRODUCTION

Tomato is one of the most important vegetable crops in the world. It belongs to the family Solanaceae, genus *Lycopersicon*, which is relatively small genus within the large and diverse family consisting of approximately 90 genera. It is consumed fresh and/or as paste in all parts of the world.(Alofe CO, 1982). About 160 million tonnes of fresh tomatoes are produced from 4.7 million ha (Faostat, 2011) wherein

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Comparative study of reproductive biology in Solanum melongena L. using different fertilizers

Arpana A Rathod, Dr. Meghna R Adhvaryu*

Department of Botany, Government Science College, Vankal, Ta. Mangrol, Surat, Gujarat, India

Abstract

Reproductive biology provides information on life forms like rate of flowering, type of breeding system, plant-pollinators interaction, fruit and seed output, overall fitness and survival of the species. Present work has been focused to determine the effects of synthetic and organic fertilizers application on the growth parameters like stage of plant development, plant height, number of leaves, number of flowers, flowers to fruits conversion and %yield. Field experiments were conducted in the farms located in *Jahangirabad* area of Surat city from 2017 to 2018. Season for experiments was chosen between month of October to April where average low temperature of Surat ranges from 15°C-21°C and average high temperature ranges from 25°C-35°C. The treatments consisted of two different fertilizers namely synthetic inorganic fertilizer (SF) consisting of NPK and organic fertilizer (OF) chiefly consisting of cow-dung/buffalo-dung/poultry manure. Three plot of 30 x 02 sq. ft area was selected to grow 30 plants of Brinjal. One plot was designated as Control group where no pre-treatment (CB group), one plot treated with SF viz. NPK (SFB group) and the other with OF (OFB group). Results suggest that OF treated plant showed increased plant height, quantity of leaves (per branch & plant) and its weight (fresh & dry), quantity of flowers and fruits, diameter and length of fruit, quantity and weight of seed per fruit as compared to Control group and well comparable with SF treatment. Thus, it is concluded that use of organic fertilizer is equally beneficial as compared to the inorganic fertilizer.

Keywords: reproductive, fertilizer, organic, inorganic, brinjal

Introduction

India is a horticultural paradise (Saravaiya SN and Patel MB, 2005) ^[15] with a vast array of vegetables being cultivated in a country wherein brinjal is one of the leading and the second major vegetable crops next to tomato which is belongs to the family Solanaceae and is known as under the botanical name Solanum melongena L. It is highly productive and usually finds a place as "poor man's crop". The young and almost mature fruit are eaten raw or used as vegetable (Edmond JB, 1985)^[6] Purple fruits have higher amino acid content. Brinjal fruits have medicinal properties (Rajan S and Markose BL, 2002)^[13] viz. use of eggplant tissues and extract include treatment of diabetes, asthama, cholera, bronchitis and diarrhea, its fruit and leaves are reported to lower certain levels of blood cholesterol. The growth, yield and fruit quality of brinjal are largely dependent on a number of interacting factors.

Reproductive biology has important consequences for the viability of rare plant populations through its effects on demography and population genetics, so its study is also crucial in conservation programs (Synge H (ed), 1981)^[16] (De Mauro MM, 1993)^[3] (weller SG, 1994)^[18] (Evans MEK, 2003). Reproduction is the life process which ensures the perpetuation of life and genetic diversity is mainly generated through recombination processes in sexual reproduction, which is, hence, a process of fundamental importance for population and species biology (Mayyard SJ, 1978)^[9].

For successful cultivation and conservation of plants a detailed knowledge of their reproductive biology is required. (Moza MK and Bhatnagar AK, 2007) ^[10]. Reproductive biology mainly focuses on flowering

phenology, floral biology, pollen pollinator interaction, breeding systems and gene flow through pollen and seeds. The task of plant phenology is to observe and record the periodically recurring growth stages and to study the regularities and dependency of the yearly cycles of development on environmental conditions.

Organic manure application is known to supply plant nutrients and improve the soil structure. It has been reported that application of organic manure showed a significant (p=0.05) increase in yield than inorganic manure in eggplant production (Ullah MS *et al.* 2008) ^[17] (Anoop and Chaubanan, 2009). The use of organic manure as fertilizer is essential in improving soil productivity and crop production (Dikinya *et al.*2010) ^[5]. The rate of organic manure application has been shown to influence growth and yield of plants (Offiong *et al.* 2010).

Present study is designed to determine the effects of synthetic inorganic fertilizers and organic fertilizers application on the growth of brinjal plant by monitoring of parameters like stage of plant development, plant height, number of leaves per branch & plant, leaves weight (fresh & dry), number of flowers, number of fruit, diameter and length of fruit, fruit weight (fresh & dry), number of seed per fruit and its weight etc.

Material and method Study area

Field experiments were conducted in the farms located in Jahangirabad area of Surat city from 2017 to 2018. Three plots of 30 x 02 sq. ft. area were selected. Soil of selected plots was tested for pH, Electrical conductivity, TOC, N, P, and K before the study started.