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Ministry of Higher Education
And Scientific Research
University of Diyala
College of Science
Department of Chemistry

Synthesis, characterization of some heterocyclic compounds and study their liquid crystalline properties

A Thesis

Submitted to the College of Science - the University of Diyala as a Partial Fulfillment of the Requirements for the Master’s Degree of Sciences in Chemistry

By

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ABSTRACT

A series of new and highly efficient heterocyclic organic compounds containing 1,2,4-triazole and thiazole rings in their structure were studied and synthesized. These compounds incorporate Schiff bases and azo dyes and are linked to alkoxy chains of different lengths in order to investigate the effect of chemical structure on the physical properties and liquid crystalline behavior of these compounds. Therefore, in order to verify the research objectives, an experimental methodology was adopted that included the synthesis of the compounds through multistep synthetic pathways, involving the formation of Schiff bases, the preparation of triazole and thiazole rings, the performance of diazotization and azo-coupling reactions, as well as the introduction of flexible alkoxy chains. Subsequently, the synthesized compounds were characterized using a range of spectroscopic and physical techniques, including fourier transform infrared spectroscopy (FTIR), proton and carbon nuclear magnetic resonance spectroscopy (^{1}H NMR and ^{13}C NMR), melting point determination, and Thin-layer chromatography (TLC) to monitor the reactions and assess purity.

The results demonstrated the successful synthesis of the compounds and the consistency of the proposed chemical structures with the obtained spectroscopic data. The study of liquid crystalline properties using polarized optical microscopy (POM) revealed that some compounds (LOC1, LOC2, and LOD3) exhibited stable nematic and smectic phases, whereas LPD2 showed a nematic phase and smectic_C and smectic_B phases. In contrast, LPE1 exhibited only a nematic phase.

These results indicate that the mesomorphic behavior of the compounds depends directly on the nature of the heterocyclic ring, the length of the alkoxy chain, and the type of substituent groups. In addition, the synthesized

compounds exhibit promising physical properties. In addition, the results obtained using an LCR meter showed variations in both the real dielectric constant (ε′) and the alternating current electrical conductivity (σ_ac) with frequency for the (LC/PMMA) compounds. It was observed that the ε′ values decreased, while the σ_ac values increased with increasing frequency for all samples. As for the standard sample (PMMA), it exhibited the lowest values, while the compounds containing liquid crystals showed higher values, particularly the compound (LPD2), which displayed the highest ε′, and (LPE1) the ε'' value. Meanwhile, (LOC2) and (LPE1) showed the highest alternating current conductivity values, followed by (LOC1) and (LPD2), whereas (LOD3) recorded relatively lower values.

Finally, it can be concluded that this behavior is attributed to enhanced polarization and charge carrier mobility in the presence of liquid crystals within the compounds. This highlights the importance of structural modification as an effective approach for developing new materials with potential applications in the field of liquid crystals and advanced functional materials.

Chapter One

Introduction

1.1 Heterocyclic compounds

Heterocyclic compounds are considered one of the most structurally diverse and pharmacologically important classes. Nowadays, the demand for these compounds is steadily increasing due to their wide synthetic and biological applications, as well as their presence in numerous natural products such as alkaloids, herbicides, vitamins, antibiotics, hormones, and pharmaceuticals. However, the synthesis of such molecules continues to pose significant challenges from both industrial and academic perspectives. All these systems have been used for the composition of unusual drugs, heterocyclic compounds have gained significant attention in both research and application [1]. The chemistry of heterocyclic compounds is an important field of modern organic chemistry [2]. As demonstrated by several molecules, a small ring system can contain one, two, or more heteroatoms. These heterocycles can be further classified into aromatic and non-aromatic. Depending on the heteroatoms present and their positions in the ring, Show in the figure (1.1) [3].

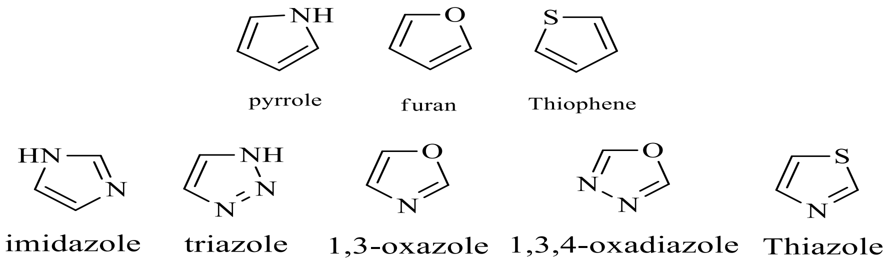


Figure 1.1: Common heterocyclic rings.

For example, Triazole is an important heterocyclic moiety that occupies a unique position in heterocyclic chemistry. Bladin first used triazole in 1855 for describing the carbon–nitrogen ring system $C_2H_3N_3$. It is a white to pale yellow crystalline solid with a weak, characteristic odour, soluble in water and alcohol [4], [5]. 1,2,4-triazoles have attracted significant interest due to their diverse structural features and wide range of biological activities, with theoretical and practical applications. Due to their unique properties in recent decades, 1,2,4-

triazoles have become one of the most sought-after topics for study in the chemistry of heterocyclic compounds. As a result, researchers have developed innovative 1,2,4-triazole derivatives exhibiting diverse structural features that facilitate the synthesis of molecules with potential antibacterial, antifungal, antitubercular, antioxidant, and anticancer activities. These derivatives are utilized in industrial, agricultural, medical, and veterinary domains. They have been used as fungicides, photosensitisers, dyes, corrosion inhibitors, and plant growth regulators, among other applications [6].

Heterocyclic composites have numerous scientific uses, and particularly five-membered heterocyclic ring-containing liquid crystalline substances have been effectively tested [7]. Soft materials involving supramolecular assembly of molecules are presently a topic of great attention in areas that range from biology and chemistry to material science. Amongst numerous soft materials, liquid crystals (LCs) are self-assembled materials that have earned great responsiveness owing to their immense technological significance, ranging from simple wristwatches to light-emitting diodes, organic field-emitting transistors, organic photovoltaic cells, etc. LCs comprising flexibility as well as order at the molecular level have found wide application in various fields like electro-optical devices and in molecular engineering nanotechnologies. LCs are unique materials which possess flow properties (e.g. fluidity, inability to support shear, formation and coalescence of droplets) of the liquids. Some layering order and features of crystalline solids (anisotropy in electrical, optical and magnetic properties, episodic alignment of molecules in one spatial direction, etc.). The main criteria for a molecule to exhibit LC behavior are:

i) It should have an elongated shape where the length must be much greater than the width.

ii) It must contain a solid core or hard nucleus.

iii) To form on flexible peripheral areas.

flexible terminal regions. The self-assembly in LCs arise from the preferred alignment of the molecules with each other because of strong intermolecular attractions [8].

Schiff bases have various applications across various fields, including analytical, inorganic, and organic chemistry. These versatile compounds are utilised as dyes, catalysts, polymer stabilisers, and luminescent chemical sensors. In addition, catalysts in CO2 fixation. They also serve as bio-lubricant additives. Several proposals have been made. For use in solar energy applications [9]. Schiff bases are a large group of compounds defined by a double bond between carbon and nitrogen atoms. Their versatility stems from the numerous ways alkyl or aryl substituents are present. These compounds can be found both in nature and synthesised in the laboratory. Over the years, Schiff bases have been a significant source of inspiration for chemists and biochemists alike [10].

Azo–Schiff base derivatives have been widely studied as thermotropic liquid crystal (TLCs) mesogens because the azo (–N=N–) and imine (–C=N–) linkages create extended conjugation and linear anisotropic shapes that favor mesophase formation. Several structural factors consistently control mesomorphic behavior: the length and parity of terminal alkyl/alkoxy chains, the presence and position of lateral or terminal polar substituents, and the nature of linking groups (azo vs. ester vs. Schiff base). Reviews and systematic studies show that introducing azo and Schiff-base moieties into a single molecule often increases polarizability and can broaden mesophase ranges, but the exact phase type nematic (Nm), smectic (Sm) depends sensitively on molecular curvature and packing [11].

Despite extensive research on heterocyclic compounds, there remains significant interest in developing new 1,2,4-triazole derivatives due to their unique biological and industrial potential. Therefore, this study aims to synthesise and investigate novel triazole-based compounds that could contribute to future advancements in material sciences.

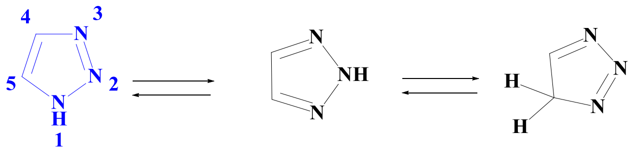
1.2 Triazole

Triazoles represent a prominent class of five-membered heterocyclic compounds containing two carbon atoms and three nitrogen atoms, with the molecular formula $C_2H_3N_3$. These rings exhibit two main positional isomers based on the arrangement of nitrogen atoms within the ring: 1,2,3-triazole and 1,2,4-triazole, Show in the figure (1.2) [12].

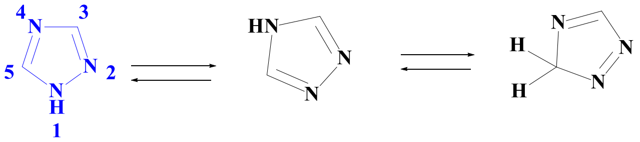
1 **1,2,3-triazole** **2** **1,2,4-triazole**

Figure 1.2: Chemical structure and numbering of 1,2,3-triazole and 1,2,4-triazole.

Triazole, also introduced as pyrrodiazole with a five-membered di-unsaturated ring skeleton, consists of two carbon atoms and three nitrogen atoms at non-adjacent sites. Each compound exists in three tautomeric forms (1a–c and 2a–c), which vary because of hydrogen bonding at nitrogen sites. In the case of 1,2,4-triazole, the 1H-1,2,4-triazole tautomer (2a) is more stable than the 4H-1,2,4-triazole tautomer (2b), as demonstrated in Figure (1.3) [13].



1H-1,2,3 triazole 1a **2H-1,2,3-triazole 1b** **4H-1,2,3-triazole 1c**



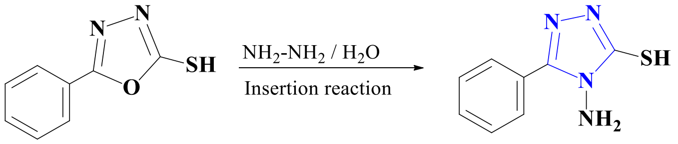
1H-1,2,4-triazole 2a **4H-1,2,4-triazole 2b** **3H-1,2,4-triazole 2c**

Figure 1.3: The tautomers of 1,2,3-triazole and 1,2,4-triazole

In particularly, the compounds with a 1,2,4-triazole core have attracted a continuously growing interest from synthetic organic chemists and those dealing with medicinal compounds due to their versatile potential to interact with biological systems **[14]**. In the industry, the use of selected 1,2,4-triazole derivatives conferred good stability and heat resistance in many molecular materials, as well as highlighted the corrosion-inhibiting capabilities of certain metals **[15]**.

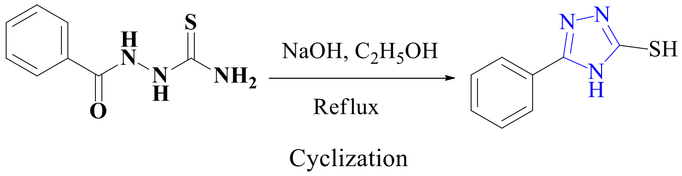
1.2.1 Conditions and Synthesis Methods of Triazole

There are several methods, such as using the Insertion reaction or the substitution reaction of the oxygen atom in oxadiazole by a sulfur atom to yield a triazole derivative: Show in the scheme (1.1)



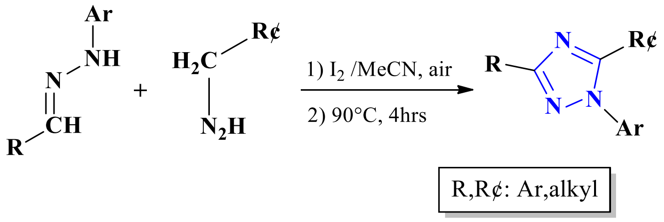
Scheme 1.1: Synthesis of the triazole derivative from substituted oxadiazole.

Another method involves the cyclization of a thiosemicarbazide derivative in a basic medium with reflux for more than 10 hrs, Show in the scheme (1.2) **[16]**.



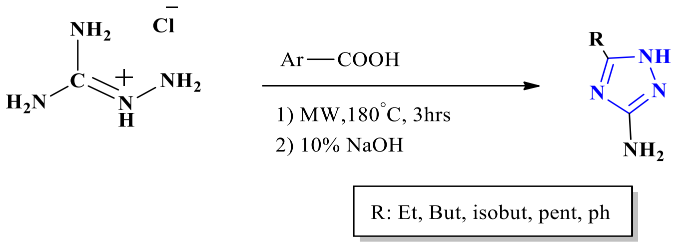
Scheme 1.2: Synthesis of the triazole derivative from cyclization.

The synthesis of 1,2,4-triazoles from aliphatic amines and hydrazones has been developed using a cascade C-H functionalization, oxidative aromatization sequence, and double C-N bond formation under iodine as the catalyst, Show in the scheme (1.3) **[17]**.



Scheme 1.3: Synthesis of the 1,2,4-triazoles from aliphatic amines and hydrazones.

A novel series of 5-substituted 3-amino-1,2,4-triazole was synthesised through the direct condensation of carboxylic acids with amino guanidine hydrochloride Show in the scheme (1.4) [18].



Scheme 1.4: Synthesis of 5-substituted 3-amino-1,2,4-triazole.

1.2.2 Application of 1,2,4-triazoles

1,2,4-Triazoles act as important pharmacophores by interacting with the biological receptors with high affinity owing to their dipole character, hydrogen bonding capacity, rigidity, and solubility. This motif is an integral part of a variety of drugs available in clinical therapy, including:

- **Antifungal:** Triazoles are widely used as antifungal agents. Compounds like of the 2-(2,4-difluorophenyl)-1,3-di(1H-1,2,4-triazol-1-yl)propan-2ol (fluconazole), itraconazole, and voriconazole belong to this class and are used to treat fungal infections, including candidiasis, aspergillosis, and Cryptococcus's, show in the figure (1.4) [19].

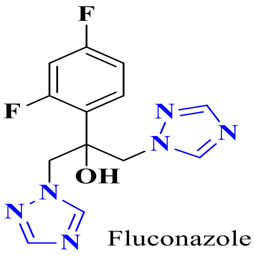

Fluconazole

Figure 1.4: Structure of fluconazole.

- **Anticancer agents:** Many chemical entities with 1,2,4-triazole motifs, such as vorozole, letrozole, 2,2-(5-((1H-1,2,4-triazol-1-yl)methyl)-1,3-phenylene)bis(2-methylpropanenitrile) (anastrozole) have emerged as promising anticancer agents, show in the figure (1.5) [20].

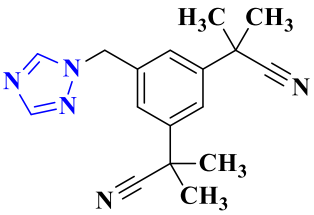

Anastrozole

Figure 1.5: Structure of the Anastrozole.

- **Antiviral agents:** triazole compounds have been shown to target a wide variety of molecular proteins, including human immunodeficiency virus (HIV), severe acute respiratory syndrome virus (SARS), hepatitis B (HBV) and hepatitis C (HCV) viruses, influenza virus, and herpes virus, and have been discovered to be susceptible to triazole derivatives, show in the figure (1.6) [21].

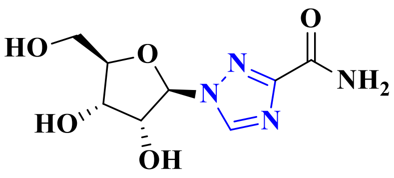

Ribavirin

Figure 1.6: Structure of the Ribavirin.

1.3 Thiazole.

The thiazole five-membered heterocyclic compound containing sulfur and nitrogen heteroatoms was first described by Hantzsch and Weber in 1887 [22]. Both an electron-donating (-S-) and an electron-accepting (-C=N-) group are present in this five-membered heterocyclic nucleus, and together they produce a stable heterocyclic molecule [23]. Thiazole-containing compounds are widely found in both natural and synthetic sources. Many thiazole-based compounds possess a broad spectrum of bioactivities. The use of thiazole derivatives in other fields, such as organic materials, cosmetics, and organic synthesis, has also been widely reported. Due to its broad applicability, the synthesis of thiazole-containing compounds has attracted extensive interest from chemists, and many studies on the synthesis of the thiazole skeleton have been reported recently [24]. These 1,3-azoles and related compounds (nitrogen and one other heteroatom in the ring) are numbered as, shown in Figure (1.7) [25].

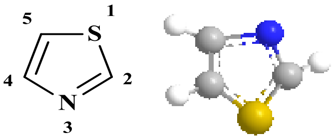
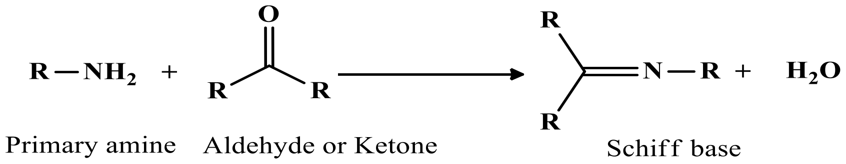


Figure 1.7: Thiazole numbering system and structure.

1.4 Schiff bases

Schiff bases are nitrogen analogues of aldehydes (R_1CHO) or ketones (R_1COR_2), in which the carbonyl group is replaced by an imine (azomethine) group (–C=N–). These compounds are typically formed by condensation between a primary amine and an aldehyde or ketone [26]. In leading to the formation of Schiff bases, aldehydes react faster than ketones because the reaction centers of aldehydes are sterically less hindered than those of ketones. Moreover, the carbonyl carbon in aldehydes typically has more partial positive charges than in ketones due to the electron-donating nature of alkyl groups. Aldehydes have only one group of electron donors, whereas ketones have two [27]. Show in the scheme (1.5) [28].

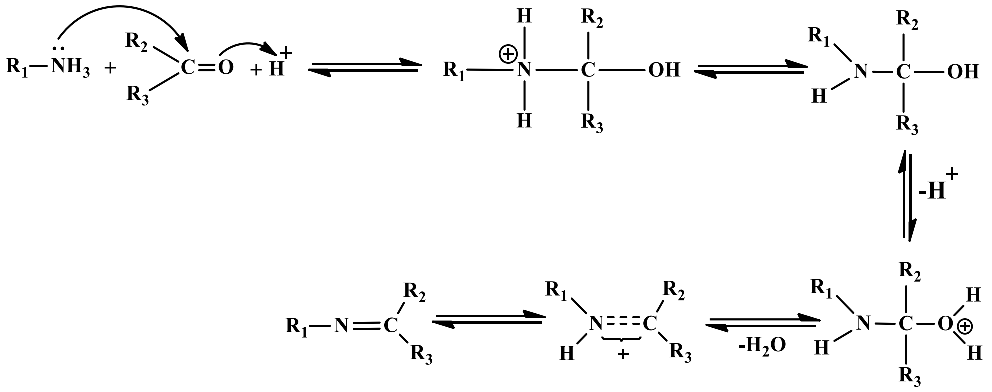


Scheme 1.5: General structure and synthesis of a Schiff base.

They are commonly represented by the general formula $R_1R_2C=NR_3$, where R_1, R_2, and R_3 can be aryl, alkyl, heteroaryl, or cycloalkyl groups. The azomethine linkage (–C=N–) plays a crucial role in the biological activity of Schiff bases. Due to their versatile structures, Schiff bases have found wide-ranging applications [26] due to their synthetic flexibility, selectivity, sensitivity to central metal atoms, and structural similarity with natural biological compounds [29]. Across various fields, including luminescent chemosensors [22], paint and polymer industries, pharmaceuticals, medicine, agriculture, and even in the formulation of rocket fuels. Furthermore, they are valuable in explaining several biological phenomena, owing to their structural diversity and chemical reactivity [30].

1.4.1 Formation mechanism of Schiff bases.

The most widely used method discovered by Schiff for the preparation of Schiff bases is the reaction of aliphatic or aromatic aldehydes or ketones with aliphatic or aromatic primary amines. The synthesis of Schiff bases obtained from the reaction of carbonyl compounds with primary amines takes place in two main steps. In the **first step**, a carbonyl amine intermediate is formed from the condensation of the carbonyl group with the primary amine, and in the **second step**, a Schiff base is formed from the dehydration of the intermediate shown in scheme (1.6) [30].



Scheme 1.6: Mechanism of condensation of carbonyl compounds with amines.

1.4.2 Synthetic methods of Schiff bases.

Numerous studies have been conducted on the synthesis of Schiff bases. Schiff bases have been prepared using conventional and green synthetic methods, show in the figure (1.8) [31].

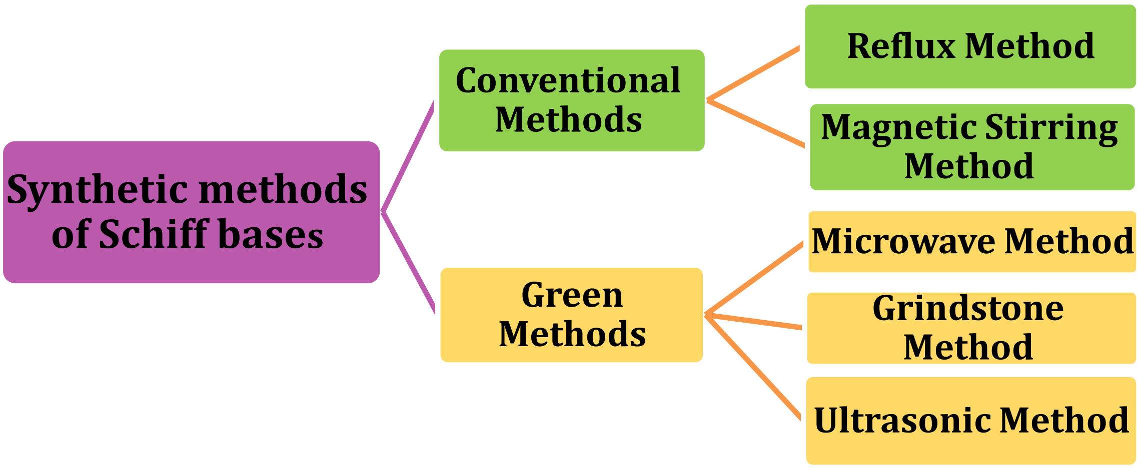


Figure 1.8: Synthetic methods of Schiff bases.

1.5 Azo Dyes

The inception of azo compounds can be traced back to 1858 when the scientist Peter Griss made the discovery. Termed as diazo compounds, Griss postulated that these compounds resulted from the replacement of two hydrogen atoms in the benzene ring by two nitrogen atoms. Subsequently, it was observed that a significant number of aromatic amines could be converted into their respective diazo compounds. In 1883, Curtin achieved the first synthesis of diazo compounds, albeit their inherent instability and rapid dissociation into nitrogen and hydrocarbons limited their prevalence when compared to aromatic azo compounds [32]. Characterised by the azo group (-N=N-), these dyes connect aromatic or aliphatic radicals and play a key role in the dyeing and printing industries, with expectations for continued growth [33]. These compounds are widely employed as colourants, contributing to approximately 50% of all synthetic dyes. Azo derivatives exhibit a broad spectrum of applications across multiple domains. Given their widespread utility, developing efficient synthetic methodologies is crucial for obtaining novel azo compounds with high yields. The most established and effective synthetic routes to azo compound preparation involve diazotisation followed by azo coupling reactions. Azo compounds possess significant biological activities, including anticancer, antifungal, antioxidant, anti-inflammatory, and antibacterial properties. Furthermore, these compounds find applications in diverse fields such as textile dyeing, printing technologies, photoelectronics, polymer modification, and materials engineering, particularly for enhancing resistance to solvents, moisture, light, and environmental degradation [34]. They are also used in paper manufacturing [35] and dye-sensitised solar cells [36]. Azo-Schiff bases can be synthesised by combining azo dyes and Schiff bases through the azomethine (C=N) bond. The integration of two chromophores into a single molecule enhances the biological and physicochemical properties of this versatile class of ligands and their metal complexes. Numerous unique synthetic azo dyes exist, including 1,2,4-triazoles, which are intriguing for several reasons. The chemistry of 1,2,4-triazoles is intricate, well-established, and stable compounds. Incorporating 1,2,4-triazole molecules has facilitated the isolation of several macro-acyclic ligands [37].

1.5.1 Classification of azo dyes

They are classified according to the number of azo groups within the molecule and include monoazoles, diazoles, ternary azo compounds, and azo compounds of higher order [35]. Furthermore, azo pigments can be classified based on the nature of the oxochromate groups embedded in them. Acidic dyes include acidic functional groups (COOH, SO3H, and OH), while basic dyes contain basic groups such as dialkyl amino, alkyl amino [38], or amino groups attached to the rings at both ends of the azo bridge [39].

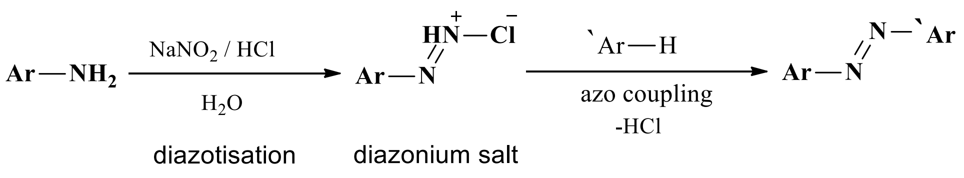
Azo compounds are characterized by the presence of the –N=N– functional group in their molecular structure, denoted as R1-N=N-R2. When the R groups in azo compounds are aromatic (arene) rings, the resulting structures exhibit enhanced stability compared to those with alkyl groups. This stability arises from the involvement of the (-N=N-) group in a wide-ranging, scattered system that includes the ring of aromatics. The aromatic azo compounds display intense coloration, making them valuable as dyes in various applications. The formation of aromatic azo compounds occurs through a coupling reaction involving the combination of a diazonium salt and a coupling agent [40].

1.5.2 Characteristics of Azo Compounds

Azo compounds are classified into two classes, depending on the rings attached to the two ends of the azo group. They are homocyclic azo compounds whose aromatic rings contain heteroatoms, such as azo benzene and its derivatives, and it is one of the most widely used classes of compounds, Azo, because of its various applications in various fields, such as the medical and industrial fields. And heterocyclic azo compounds, which contain one or both ends of the azo group on heterocyclic aromatic rings containing one or more heteroatoms (N, O, S). which are widely used as reagents in the field of analytical chemistry for spectroscopic determination of many Chemical elements. where they have received a great deal of attention due to their high selectivity and sensitivity. The azo group is characterized by having excellent donating properties due to the presence of free electrons on the nitrogen atoms of the azo group, so it is considered one of the important ligands in coordination chemistry. The azo group (–N=N–) is one of the principal chromophores, and it is responsible for the coloration of azo compounds. In addition, azo compounds may contain auxochromic groups and other substituents that not only intensify color but also improve solubility, selectivity, and sensitivity in both the compounds and their metal complexes. The azo group is one of the three chemical groups that are considered the most common and used in the production of dyes, namely (Azo group, phthalocyanine, anthraquinone), and is the most important as it represents the main class of synthetic dyes. Azo compounds have bright colors of high intensity, as their colors range from (yellow - orange- Red - green - to blue) According to the structure of the molecule **[41]**.

1.5.3 Synthesis of azo dyes

The two-stage reaction pathway comprising diazotisation and azo coupling is depicted in Scheme (1.7). The initial phase of diazotisation entails the reaction of a primary aromatic amine (Ar-NH_2), known as the diazo component, with $NaNO_2$ under regulated acidic conditions and at low temperatures (0-5°C) to produce a diazonium salt (Ar-N^+Cl^-). In the second step of the process, azo coupling, the more unstable diazonium salt reacts with a coupling component, which may be a phenol, an aromatic amine, or a β-ketoacid derivative, to produce the Azo dye or pigment **[42]**.



Scheme 1.7: Diazotization and azo coupling.

1.5.4 Applications for Azo Dyes

Azo dyes are widely used in various industries, including printing, textiles, fiber, leather, cosmetics, and paint. In addition to their role in colouring, azo compounds have been demonstrated to have cytotoxic, antiviral, antifungal, and antibacterial qualities [34]. The azo dyes have low cost, high intensity, and colour fastness, which has led to them being the most frequently used class of dyes (~60%) [43].

This study focuses on the innovative design and synthesis of novel Azo-Schiff bases incorporating 1,2,4-triazole moieties, aiming to explore their unique physicochemical characteristics and evaluate their potential biological applications. Among the expected results are the creation of structurally varied compounds with improved activity and stability. Contributing to the development of industry and materials science

1.6 Liquid crystals

Liquid crystals (LCs) represent an intermediate state of matter. They lie between the regular crystalline solid, in which particles are restricted in movement and arranged in a three-dimensional lattice, and the irregular liquid, in which particles move randomly [44]. Thus, liquid crystals exhibit anisotropy similar to crystalline solids, while also retaining the fluidity of isotropic liquids [45]. (LCs) Technology has a well-established history of applications in visible light, particularly in the display industry [46]. LCs, also with their unique ordered mesophases and anisotropic physical properties, such as optical, magnetic, and dielectric anisotropies, have found wide optoelectronic applications, especially liquid crystal displays (LCDs) in digital electronic devices, such as smartphones, tablets, laptops, TVs, etc. LCs incorporating 2,5-disubstituted pyrimidine rings in their aromatic cores are often used in commercial LCDs, show in the figure (1.9) [47].

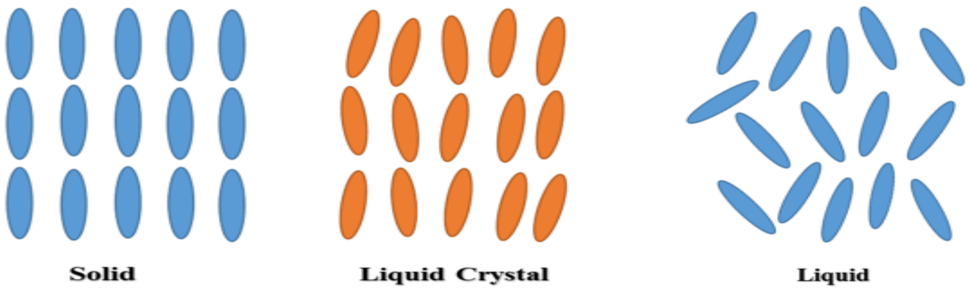


Figure 1.9: Molecular of liquid crystals in solid and liquid states.

LCs have been the subject of study for fundamental science and in many fields of research, such as chemistry, physics, medicine, and engineering, which have contributed to the progress in materials science and to innovative applications. Compared to other solid-state materials, LCs present unique attributes because they easily respond to external stimuli such as surfaces, light, heat, mechanical force, or electric and magnetic fields, and eliminate defects by self-healing. Thus, the understanding of the relationship between the chemical structures of liquid crystalline compounds and their specific functions is becoming more important **[48]**.

1.6.1 Classification of liquid crystal

LCs can be classified based on the formation of the mesophase, which depends on the concentration in a given solution (lyotropic) or by varying the temperature (thermotropic). Among thermotropic liquid crystals (TLCs), there is a further distinction based on whether the LC behaviour is observed in one direction, either cooling or heating (known as monotropic), or in both heating and cooling (known as enantiotropic). In addition, they can also be classified based on the shape of the molecule (rod-like, disc-like, bent-core, etc.) and the organization in the liquid crystalline phase (Sm, columnar, (Nm), cholesteric, blue phases, etc. show in the figure (1.10) **[49]**.

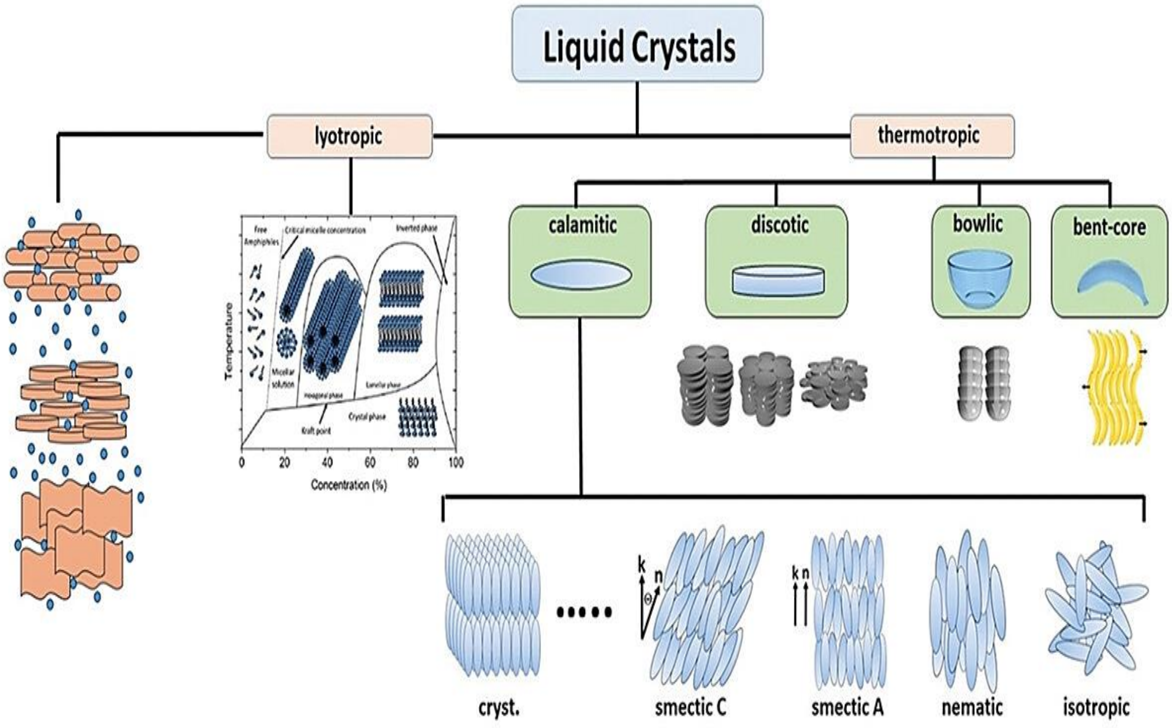


Figure 1.10: General classification of liquid crystals.

1.6.1.1 Thermotropic Liquid Crystals

In TLCs, phase transitions are governed by temperature as a fundamental thermodynamic control parameter. These transitions can be initiated by heating a crystalline solid (either pure compound or compound mixtures) and by cooling an isotropic liquid. TLCs are built up by individual molecules, and no further molecular species (specifically solvents) are required for the LC phase formation . At the heart of TLCs are chemical structures – mesogenic cores, also known as mesogens. These cores exhibit specific molecular shapes and functionalities that define the liquid crystalline behavior. Common examples include aromatic rings, biphenyls, and other rigid units. The type and arrangement of mesogenic cores heavily influence the phase behavior and physical properties of TLCs [50].

TLCs are extensively recognised due to their applications in television, laptop, mobile phone, and tablet displays, according to their structural features [51]. Mesophases of such LCs can be divided into categories that depend on the orientation and order. The main categories are (Nm), Sm, and cholesteric (Nm) or chiral (Nm) [52].

1.6.1.2 Lyotropic Liquid Crystals

Mainly amphiphilic molecules that have a nonpolar head and a polar tail form Lyotropic liquid crystals (LLCs). These molecules exhibit liquid-crystalline behavior in certain solvents at specific temperatures and concentrations. LLC phases can be classified into three main groups: lamellar, columnar, or cubic phases, among others, depending on the positional order [42]. In a lyotropic liquid crystal system, the transition between mesophases depends on the solvent concentration. Besides, they can form highly stable mesophases, classified in lamellar, hexagonal, or cubic phases, according to the organization of micelles [53]. Lyotropic substances are strongly birefringent [54]. Have drawn attention in numerous technical fields as they feature a variety of nanometer-scale structures, processability, and diverse chemical functionality. However, they suffer from poor mechanical properties and thermal stability [55].

1.7 Liquid Crystal Phases

1.7.1 Nematic phases

The Nm liquid crystal phases are ubiquitous in our daily lives thanks to their widespread adoption in display technology. The (Nm) phase is characterized by its constituent molecules (or particles) having, on average, a preferred direction of orientation, which is termed the director. As with virtually all fluid phases of matter at equilibrium, the bulk (Nm) LCs we encounter day-to-day are apolar, irrespective of their molecular polarity [56]. The (Nm) liquid crystalline phase is technologically the most important of the well-known and widely studied mesophases. (NM's) are also the most used, because they illustrate the best dual nature of LCs. Hence, the molecules that form LC mesophases display a unique combination of properties between long-range order and mobility, the basis of the numerous technical applications. These elongated molecules have randomly oriented centers of mass and directed long axes. Although they show long-range orientational order, they lack long-range positional order. LCD displays and other display technologies frequently use (Nm) LCDs, show in the figure (1.11) **[57]**.

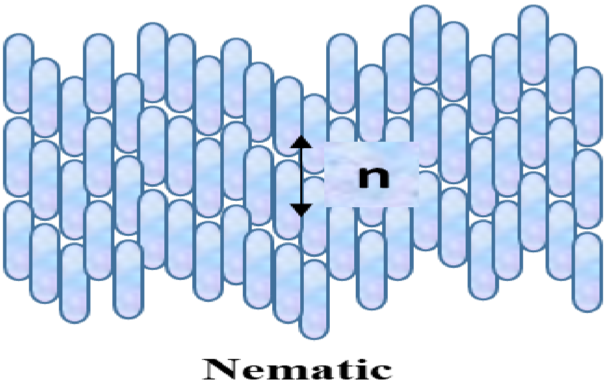


Figure 1.11: The (Nm) liquid crystal phases.

1.7.2 Smectic phase

The Sm phase is the phase that looks most like a crystalline solid, and for which molecules ordered in equidistant layers. It shows a long-range positional order (at least in one direction) and an orientational order in each layer. An additional degree of order, the layered structure characterizes it. This phase is more viscous and occurs at a lower temperature. The most common Sm phases are (SmA), in which the molecules orient perpendicular to the layer plane, and (SmC) phases, where the molecules are tilted with respect to the layers **[58]**. As shown in the schematic illustration of the SmA and smC phases. In SmA, the orientation of LC molecules **n** is well defined; they align along the layer normal **m**, resulting in a layer structure. In SmC, the orientation of molecules **n** deviates from the layer normal **m,** show in the figure (1.12) **[59]**.

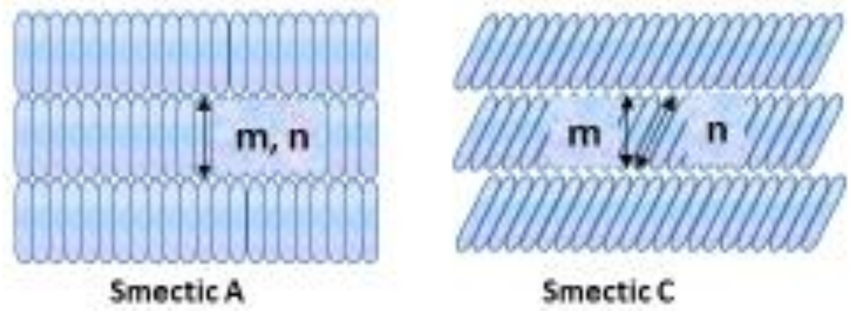


Figure 1.12: The SmA and SmC liquid crystal phases.

1.7.3 Cholesteric phases

Configuration is precisely like the nematic phase obtained by winding the nematic about the x-axis which was originally aligned along the y axis. The spiral arrangement thus formed is accountable for the typical colors of cholesterics in reflection as well as their very huge rotatory power. Similar to nematics, it displays long-range orientation order and no positional alignment and diverges from the nematic phase wherein the director differs in direction all through the medium in a regular way. There is no phase changeover between nematic and cholesteric phases in a given material. The molecules developing this phase areal ways optically active. Fingerprint and Grandjean or standing helix textures are the most observed cholesteric textures, shows in the figure (1.13) **[60]**.

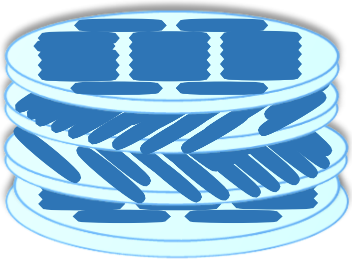


Figure 1.13: The Cholesteric liquid crystal phases.

1.7.4 Columnar phases

Disk-shaped mesogens can orient themselves to pack into stacks in a layer-like fashion to form discotic columnar phases. The columnar phases with long-range order can be organized mainly as rectangular or hexagonal arrays, show in the figure (1.14) [61].

Figure 1.14: The Columnar liquid crystal phases.

1.8 Applications of Liquid Crystals

(LCs) have been considered peculiar substances since their discovery in 1888. The demand for low-power, high-efficiency displays has invigorated research into (LC) electro-optical characteristics, offering a wide range of applications beyond displays, including switchable windows, thermometers, plasmonics, photovoltaics, and solar cells. This section is devoted to exploring some practical and novel applications of LCs in different areas of day-to-day life, as summarized in Figure (1.15) [54].

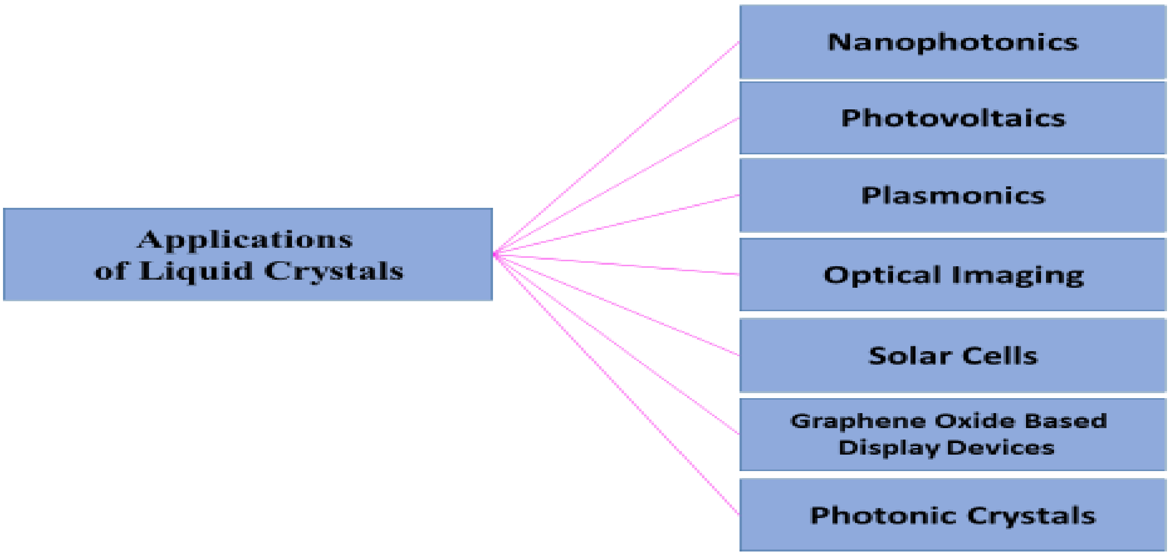


Figure 1.15: Application of the liquid crystal research.

LCs are an important topic of research not only because of their enormous variety of applications but also because they provide a platform for addressing a variety of fundamental problems in physics. The Nm phase is extensively used in LCDs, and the search for newer LCs with improved sensitivity and stability remains an ongoing activity [62].

The aim of the study

1. Preparation of heterogeneous cyclic compounds derived from the amino acid (Glycine).
2. Preparation of a series of azo compounds derived from the compound prepared in the first step.
3. Preparation of a series of azo compounds derived from (2-amino-4,5-dimethylthiazole).
4. Preparation of a series of Schiff base compounds derived from the compound (2-aminothiazole).
5. Preparation of new ethers derived from the synthesised compounds, containing five and eight carbon aliphatic chains.
6. Study of the liquid crystalline properties of the prepared compounds.
7. Study of the electrical properties of prepared compounds that possess liquid crystalline characteristics.

وزارة التعليم العالي والبحث العلمي
جامعة ديالى
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قسم الكيمياء

تحضير وتشخيص بعض المركبات الحلقية غير المتجانسة ودراسة خصائصها البلورية السائلة

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مجلس كلية العلوم - جامعة ديالى
كجزء من متطلبات نيل درجه الماجستير
في علوم الكيمياء

من قبل

حنين جابر عطيوس
بكالوريوس علوم كيمياء 2021
كلية العلوم - جامعة ديالى

بأشراف

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أستاذ مساعد. د. نور صباح أحمد

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