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Effect of mesogenic linkages on two novel aromatic series-based liquid crystals: synthesis, theoretical and comparative studies

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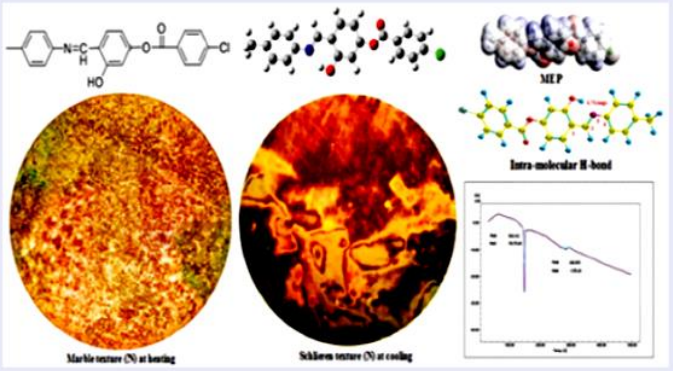
ABSTRACT

Two novel groups of rod-like homologue molecules, one group (group **A**) having benzothiazole-aromatic mesogenic units and the other (group **B**) with only aromatic mesogenic units, were designed and synthesised. Both groups (compounds **A** and **B**) involve azomethine (–CH=N–), ester (–COO–), azo (–N=N–) and amide (–NH–CO–) linking groups at the different positions in their molecular structures. The structures of the synthesised compounds were elucidated using different analytical techniques (^{1}H, ^{13}C NMR, FT–IR, mass spectra and melting points). In order to verify the influence of the central linkages and their positions on physicothermal and mesomorphic properties, different types of linking groups including –CH=N–, –COO-, –N=N– and –NH–CO– were analytically and thermally investigated. Thermal analyses and mesomorphic properties of both series are discussed in terms of the linkages nature, comprising geometrical structure, interactions polarisability, subtle change in shape and their effective positions. The results revealed that the synthesised compounds (groups **A** and **B**) showed the only enantiotropic nematic mesophase in certain temperature regions except compounds **A4** and **A6**. The change of the type linkages and their positions in some compounds (groups **A** and **B**) was theoretically investigated to verify if the theoretical calculations show an agreement with the experimental findings.



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Introduction

The particular properties shown by liquid crystal (LC) molecules inspire many researchers to design a large number of analogous molecules and investigate their mesomorphic properties that have yet to be structurally determined [1,2]. In the display area, LC molecules play a key role in many applications such as information storage, photoelectric devices, mobile telecommunication, biomedical diagnosis, computing devices and optical storage [3–5]. The majority of LC molecules utilised in the abovementioned applications contain rod-like molecules [6,7]. Thus, it is a challenging task for researchers to design rod-like molecules with the required modification or functionalization without losing their liquid crystalline behaviours and enhance new added values towards their potential applications [8–10]. Molecular structure-relationship and nature of linking spaces are essential factors for LC molecules [11,12]. To identify appropriate molecular structures for showing desired liquid crystalline behaviours, the candidate molecules should have linear, rigid and dipole structures [13]. Two types of dipoles accompany with these molecules: the first strong one occurs towards the centre molecules and the other weak one in the end [14]. In the rod-like molecules, the

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