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# Synthesis, mesomorphic properties, and theoretical study of benzothiazole-aromatic molecules with ester- and azomethine-linking groups

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#### ABSTRACT

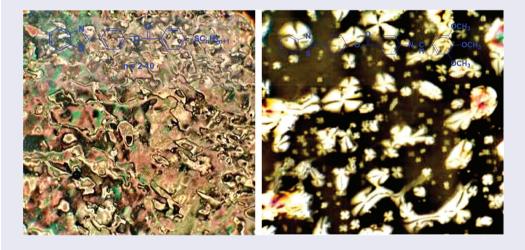
Two novel groups of rod-like molecules with benzothiazole-aromatic systems: one group (group A) having an ester linkage with different thioalkyl chain length and the other (group B) ester- and azomethine-linkages with methoxy groups in the tip of the molecules were synthesised. The structures of the synthesised compounds were confirmed by using physicochemical techniques such as <sup>1</sup>H NMR, mass spectra, FT-IR spectra, melting points, and elemental analyses. Differential scanning calorimeter and polarising optical microscopy have been employed to verify their liquid crystalline behaviours and transition temperatures. All the synthesised compounds (groups A and B) showed enantiotropic nematic phase except the compound 13d showed the nematic phase in cooling only. The mesomorphic properties of the present compounds were compared with some other structurally related compounds to understand the chemical structure–mesophase properties relationship. The thermal range of nematic phase for the compounds (group A) were decreased with the increase of the thioalkyl chain length. The liquid crystalline properties of the compounds (group B) were greatly affected by the position of terminal methoxy groups. The change of the position of terminal methoxy groups in the compounds (group B) was theoretically studied to investigate if the theoretical calculations possess an agreement with the practical results.

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Benzothiazole liquid crystals; terminal thioalkyl chain; linking groups; ester; azomethine; theoretical study



# Introduction

The fascinating behaviour of rod-like liquid crystal molecules, in which they are used in LCD technology, photoelectric devices, biomedical diagnosis, sensors, and information storage units [1,2]. The rod-like liquid crystals also offer foreseeable applications as they can be employed in reflective liquid crystal displays, including computing devices, holographic media [3], mobile telecommunication, reversible optical waveguides [4], and photo-alignment of LC systems [5]. The liquid crystal molecules that have a rod-like shape are usually combined with the major dependence of the essential properties involving molecular structure nature, type of linking groups, terminal substitution, and chemical constitution [6]. The formation of the thermotropic liquid crystal molecules with rod-like shape and linear structure, these molecules are generally required to have certain rigid structures. The molecules that exhibit liquid crystalline behaviour possess dipoles in their structures: the first dipole is strong towards the centre and the other is weak towards the end of the