Indian Journal of Heterocyclic Chemistry
Vol. 35 - Number 04 (Oct-Dec 2025) 875-881
https://connectjournals.com/01951.2025.35.875
https://doi.org/10.59467/IJHC.2025.35.875

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Synthesis of new Symmetric dimers derived from benzothiazole, and study of their liquid crystalline properties supported by theoretical calculations

Hayder Hami Gitr*, Uhood J. Al-Hamdanib and Adil Muala Dhumad
Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, Iraq

ABSTRACT In this study, two new dimers (dimer **1**, [*N,N'*-(((octane-1,8-diylbis(oxy))bis(4,1-phenylene)) bis(methanylylidene))bis(benzo[d]thiazol-2-amine)]) (H-O8O-H) and (dimer **2**, [*N,N'*-(((octane-1,8-diylbis(oxy)) bis(4,1 phenylene))bis (methanylylidene)) bis-(6-chlorobenzo[d]thiazol-2-amine)]) (Cl-O8O-Cl) were synthesized. The synthetic approach involved two steps: i) preparation of dialkoxy dimer by the reaction of octyl bromide with *para*-hydroxybenzaldehyde, and ii) conversion of dialkoxy dimer to the target dimers (Schiff bases) by the reaction with 2-aminobenzothiazoles. Differential scanning calorimetry (DSC) and polarized optical microscopy (POM) were used to look at the mesomorphic properties of the two dimers. DSC and POM analysis indicated that the dimer **1** did not show any liquid crystalline phase, while the dimer **2** substituted with Cl showed only the nematic phase. The thermal and geometrical parameters of the dimers under investigation were assessed using density functional theory to determine the alignment of theoretical calculations with empirical results. The dimer **2** has a high transition temperature and can be employed in industries that demand liquid crystalline phases at elevated temperatures.

KEYWORDS Liquid crystal, Dimer, Nematic, Schiff base.

How to cite this article: Gitr, H.H., Al-Hamdanib, U.J. and Dhumad, A.M. Synthesis of new Symmetric dimers derived from benzothiazole, and study of their liquid crystalline properties supported by theoretical calculations, *Indian J. Heterocycl. Chem.*, **2025**, *35*, 875–881. *https://doi.org/10.59467/IJHC.2025.35.875*