Journal of Molecular Liquids 414 (2024) 126272

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Structural analysis and theoretical studies of 2-(2-chlorobenzylidene) malononitrile (CS) "a riot controlling agent"

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ARTICLE INFO

Keywords:
X-ray diffraction
Hirshfeld surface
DFT studies
PASS
Docking

ABSTRACT

In solvent methanol, malononitrile and 2-chlorobenzaldehyde were stirred in the presence of base piperidine to synthesise the target chemical 2-(2-chlorobenzylidene) malononitrile (CS). The crystal structure of the target compound $C_{10}H_5ClN_2$ has been elucidated through X-ray crystallographic analysis. It crystallises in the monoclinic crystal system within the P21 space group, containing four molecules per asymmetric unit. The unit cell dimensions are a = 3.8825(3) Å, b = 21.0202(18) Å, c = 21.3481(18) Å, and β = 95.096(4)°. The phenyl and malononitrile groups, which make up the molecular components, are each planar but slanted towards one another at a dihedral angle of 12.7° (4). Besides this, target molecule is also stabilized by hydrogen bonding, halogen bonding and π stacking interactions. Solid-state structure has been analysed through Hirshfeld surface analysis, including the evaluation of the different energy frameworks, indicating that the molecular sheets are primarily formed by hydrogen bonds and halogen bonds and the stabilization is dominated via the electrostatic energy contribution. Fingerprint plots were carried out to study the relative contribution of noncovalent interactions in the target compound CS. Further, the density functional theory calculations were employed using B3LYP hybrid functional with 6-311++G level basic set to optimize the structural coordinates in gas phase and in different solvents (chloroform, water, and methanol). The chemically active regions of the target compound were identified by the analysis of molecular electrostatic potential surface. Further, from PASS analysis and literature reports, molecular docking of title compounds was carried out with human transient receptor potential ankyrin 1 ion channel (hTRPA1) (PDB-ID 6PQO). ΔGb (docking energy) and inhibition constant was calculated to be −7.53 kcal/mol and 3.33 μM respectively, with the target ion channel.

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https://doi.org/10.1016/j.molliq.2024.126272
Received 28 March 2024; Received in revised form 3 October 2024; Accepted 13 October 2024
Available online 16 October 2024