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Synthesis, molecular structure, Hydrogen-bonding and chemical reactivity analysis of 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(2-chlorophenyl)-dipyrrromethane: A combined experimental and theoretical approach

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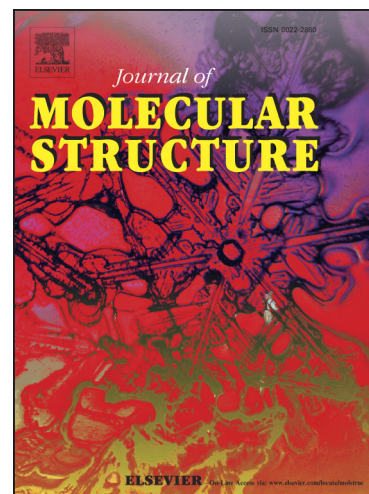
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**Synthesis, molecular structure, Hydrogen–bonding and chemical reactivity analysis of 1,9–bis(2–cyano–2–ethoxycarbonylvinyl)–5–(2–chlorophenyl)–dipyrromethane: A combined experimental and theoretical approach**

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**Abstract**

The spectroscopic analysis of a newly synthesized 1,9–bis(2–cyano–2–ethoxycarbonylvinyl)–5–(2–chlorophenyl)–dipyrromethane (**3**) has been carried out using <sup>1</sup>H NMR, UV–Visible, FT–IR and Mass spectroscopic techniques. The presence of a <sup>1</sup>H NMR signal at 5.93 ppm indicates that two pyrrole units joined together at meso position. The intense absorption in UV region at  $\lambda_{\max}$  (315nm) is caused by the excitation of electron from singly occupied molecular orbital H–1 [n(O11)] to L+1[ $\pi^*(C10–O11)$ ]. Natural bond orbitals (NBOs) analysis reveals various types of intramolecular conjugative and hyperconjugative interactions within molecule. The conjugative interactions are responsible for  $\pi$ –electron delocalization within pyrrole or benzene ring and stabilized the molecule with energy in the region 11.63–22.64 kcal/mol. A combined experimental and theoretical vibrational analysis indicates the existence of intramolecular H–bonding between pyrrole N–H as proton donor and N atom of cyanide as proton acceptor. To investigate the strength and nature of H–bonding, topological and energetic parameters at bond critical points (BCP) have been analyzed by ‘Quantum theory of Atoms in molecules’ (QTAIM). Global electrophilicity index ( $\omega = 4.58$  eV) shows that title molecule (**3**) is a strong electrophile. The maximum values of local electrophilic reactivity descriptors ( $P_k^+$ ,  $f_k^+$ ,  $\omega P_k^+$ ,  $NP_k^+$ ) at vinyl carbons (C6 / C22) of (**3**) indicate that they are more prone to nucleophilic attack.

**Keywords:** Vibrational analysis, electronic transition, NBO analysis, Hydrogen–bonding, QTAIM analysis, reactivity descriptors

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