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Quantum mechanical and spectroscopic (FT-IR,  $^{13}\text{C}$ ,  $^1\text{H}$  NMR and UV) investigations of potent antiepileptic drug 1-(4-chloro-phenyl)-3-phenyl-succinimide

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**Quantum mechanical and spectroscopic (FT-IR,  $^{13}\text{C}$ ,  $^1\text{H}$  NMR and UV) investigations of potent antiepileptic drug 1-(4-chloro-phenyl)-3-phenyl-succinimide**

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**Abstract**

This study represents an integrated approach towards understanding the vibrational, electronic, NMR, and structural aspects, and reactivity of 1-(4-chloro-phenyl)-3-phenyl-succinimide (CPPS). A detailed interpretation of the FT-IR, UV and NMR spectra were reported. The equilibrium geometry, bonding features, and harmonic vibrational frequencies have been investigated with the help of density functional theory (DFT) B3LYP method using 6-31G(d,p) and 6-311++G(d,p) basis set. The scaled theoretical wavenumber showed very good agreement with the experimental values. The  $^1\text{H}$  and  $^{13}\text{C}$  nuclear magnetic resonance (NMR) chemical shifts of the molecule were calculated by the gauge-invariant atomic orbital (GIAO) method. Stability of the molecule, arising from hyperconjugative interactions and charge delocalization, has been analyzed using natural bond orbital (NBO) analysis. The results show that ED in the  $\sigma^*$  and  $\pi^*$  antibonding orbitals and second order delocalization energies  $E(2)$  confirm the occurrence of intramolecular charge transfer (ICT) within the molecule. UV-Vis spectrum of the compound was recorded and the electronic properties, such as HOMO and LUMO energies, were calculated by Time-Dependent DFT (TD-DFT) approach. To

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