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

Vesna D. Vitnik, Željko J. Vitnik, Nebojša R. Banjac, Nataša V. Valentić, Gordana S. Uš ćumlić, Ivan O. Juranić

PII: S1386-1425(13)00847-0
DOI: http://dx.doi.org/10.1016/j.saa.2013.07.099
Reference: SAA 10843

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received Date: 16 March 2013
Revised Date: 20 July 2013
Accepted Date: 31 July 2013

Please cite this article as: V.D. Vitnik, Ž. Vitnik, Ž.R. Banjac, Ž.V. Valentić, Ž.S. Uš ćumlić, Ž.O. Juranić, Quantum mechanical and spectroscopic (FT-IR, ^{13}C, ^{1}H NMR and UV) investigations of potent antiepileptic drug 1-(4-chloro-phenyl)-3-phenyl-succinimide, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2013), doi: http://dx.doi.org/10.1016/j.saa.2013.07.099

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

Vesna D. Vitnik,[a,*] Željko J. Vitnik,[a] Nebojša R. Banjac,[b] Nataša V. Valentić[b], Gordana S. Ušćumlić[b], Ivan O. Juranić[a]

[a] *Department of Chemistry, IChTM, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia*

[b] *Department of Organic Chemistry, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia*

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}H and ^{13}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 σ* and π* 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