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PII: S1386-1425(17)30546-2
DOI: doi:10.1016/j.saa.2017.06.068
Reference: SAA 15284

To appear in:

Received date: 21 December 2016
Revised date: 5 June 2017
Accepted date: 30 June 2017

Please cite this article as: Alaaeldin M F Galal, Elsayed M. Shalaby, Ahmed Abouelsayed, Medhat A. Ibrahim, Emad Al-Ashkar, Atef G Hanna, Structure and absolute configuration of some 5-Chloro-2-methoxy-N-phenylbenzamide derivatives., (2017), doi:10.1016/j.saa.2017.06.068

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Abstract

The absolute configuration of 5-Chloro-2-methoxy-N-phenylbenzamide single crystal [compound (1)] and the effect of introducing -$[CH_2]_n$-, n=1,2 group adjacent to the amide group [compounds (2) and (3)], were studied. Furthermore, the replacement of the methoxy group with a hydroxy group [compound (4)] was defined. Proton and carbon-13 NMR spectrometer were used to record the structural information of the prepared compounds. X-ray single crystal diffractometer were used to elucidate the 3D structural configurations. Intensity data for the studied compounds were collected at room temperature. The X-ray data prove that compound (1) is almost planar, with maximum r.m.s. deviations of 0.210(3) $\AA$ corresponds to C13. This planarity starts to disturb by adding -$[CH_2]_n$-, n=1,2 groups between the NH group and the phenyl ring in compound (2) and (3), respectively. By replacing the OCH_3 group by an OH group in compound (4), the plane of the chlorophenyl moiety is nearly perpendicular to that of the phenyl ring. Such new structural configurations were further illustrated by the infrared, and ultraviolet-visible spectroscopy measurements in the frequency range 400-4000 cm^{-1} and 190-1100 nm, respectively. Spectroscopic analyses were verified with the help of molecular modeling using density functional theory. The estimated total dipole moment for the prepared compounds reflects its ability to interact with its surrounding molecules. The higher dipole moment for a given structures is combined with the higher reactivity for potential use in medicinal applications.

Keywords: `5-Chloro-2-methoxy-N-phenylbenzamide, NMR, Single crystal, FTIR, UV-Vis, Molecular Modeling.`

2010 MSC: 00-01, 99-00

1. Introduction

5-Chloro-2-methoxy-N-phenylbenzamide derivatives were chemically synthesized for possible use in pharmaceutical applications [1]. The conformation of the amide group is of prime importance in determining the backbone structure of polypeptides and proteins. The trans-planar conformation (I) of the peptide link has long been accepted as dominant in N-mono-substituted straight chain amides [2, 3] and proteins [4], whereas the cis-planar conformation (II) has been proposed [5] for some of the residues of fibrous proteins.

N-alkyl-amides, R-CONH-R', provided R and R' are not both larger than Et and i-Pr, both cis and trans conform-

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