chemistry proceedings

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A Comparative Theoretical and Spectroscopic Study of Aminomethylbenzoic Acid Derivatives as Potential NLO Candidates †

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† Presented at the 24th International Electronic Conference on Synthetic Organic Chemistry, 15 November–15 December 2020; Available online: https://ecsoc-24.sciforum.net/.

Abstract: Three aminomethylbenzoic acid derivatives were theoretically studied at M062X/6-311++G(d,p) level in a vacuum, namely 2-ammonio-5-methylcarboxybenzene perchlorate (**1**), 4-(ammoniomethyl) carboxybenzene nitrate (**2**) and 4-(ammoniomethyl)carboxybenze perchlorate (**3**). The compounds' structures were fully optimized and compared with the single-crystal X-ray diffraction results, showing a very close agreement with the experimental structural parameters. Their IR, 1H- and 13C-NMR spectra were calculated and examined in detail. Furthermore, the molecular electrostatic potential (MEP) maps of the studied compounds were investigated and the strength of the non-covalent interactions evaluated. In addition to these results, the NLO properties of the three compounds were predicted.

Keywords: aminomethylbenzoic acid derivatives; M06-2X Studies; optimized structure; FTIR; ^{1}H-NMR; ^{13}C-NMR; MEP; non-covalent interactions; hydrogen bonds; NLO properties

Citation: Direm, A.; Sayin, K. A Comparative Theoretical and Spectroscopic Study of Aminomethylbenzoic Acid Derivatives as Potential NLO Candidates. *Chem. Proc.* **2021**, *3*, 102. https://doi.org/10.3390/ecsoc-24-08099

Published: 13 November 2020

1. Introduction

2-carboxy-4-methylaniline (known as 2-amino-5-methylbenzoic acid) and 4-(aminomethyl)benzoic acid (PAMBA) are biologically active molecules serving as pharmaceutical intermediates [1] and their derivatives are considered as potential agents for anti-cancer chemotherapy and evaluated for their cytotoxic activity [2–4]. Furthermore, PAMBA, described for its antifibrinolytic action [5,6], is known with its derivatives to inhibit the proliferation of endothelial cells [7,8] and are additionally proven to be antiproteolytic [9].

A structural survey associated with 2-carboxy-4-methylanilinium derivatives and their related amino acids in the structural database (CSD, Version 5.39 [10]) returned only two hits, namely: 2-carboxy-4-methylanilinium perchlorate (**1**) (CSD refcode: CURKOR [11]) and 2-carboxy-4-methylanilinium chloride monohydrate (CSD refcode: GAZZAK [12]). Furthermore, the zwitterionic form of 4-(aminomethyl)benzoic acid, viz. 4-(ammoniomethyl)benzoate monohydrate (CSD refcode: PONTAP), was reported once in the literature [13], and the database survey showed two hits of (4-carboxyphenyl)methanaminium salts (the nitrate derivative (**2**), CSD refcode: CURCUX and the perchlorate salt (**3**), CSD refcode: CURLAE) [11].

Quantum chemical calculations have been considered an attractive research area in the last few years [14–17]. Therefore, modelling studies of the salts (1)–(3) were carried out by using the M06-2X with a 6-311++G(d,p) basis set in the gas phase and the struc-