



# Ionization of vitamin C in gas phase: Theoretical study

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## ABSTRACT

In this work, the gas phase ionization energies and photoelectron spectra of four important conformers of vitamin C were calculated. Symmetry adapted cluster/configuration interaction methodology employing the single and double excitation operators (SAC-CI SD-R) along with D95++(d,p) basis set were used for the calculations. Thermochemistry calculations were also performed on all possible conformers of vitamin C to find the relative stability of conformers in the gas phase. The calculated ionization bands of each conformer were assigned by calculating the contribution of natural bonding orbital (NBO) in the calculated canonical molecular orbitals involved in the ionization. SAC-CI calculations showed that the first ionization band of vitamin C is related to the  $\pi$  electrons of C=C bond of the ring of molecule although, there is the lone electron pairs of oxygen atoms and  $\pi$  electrons of C=O bond in the molecule.

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## 1. Introduction

Vitamins are classified into two groups including fat-soluble (A, K and E) and water-soluble light sensitive (C, B<sub>2</sub>, B<sub>12</sub>, B<sub>6</sub> and B<sub>9</sub>) vitamins [1,2]. Vitamin C is the most effective nutrients for human's health [3] and is present in many different forms i.e. ascorbic acid, dehydroascorbic acid, calcium ascorbate, magnesium ascorbate, chromium ascorbate, potassium ascorbate, molybdenum ascorbate, zinc ascorbate, sodium ascorbate, ascorbyl palmitate and ester C [4]. Antioxidant properties of vitamin C protect cells and DNA from damage and mutation [5,6]. Vitamin C also protects our health from the risks such as cardiovascular, cancer, stroke, eye health and immunity to live longer.

One of the most important processes, which can take place when biomolecule irradiated by the light with sufficient energy, is ionization. Ionization changes the geometry of the produced ion compared to the neutral molecule and sometimes is accompanied by molecular fragmentation and production of smaller ions, neutral radicals and ballistic secondary electrons which alter the surrounding matter [7,8,9,10,11,12,13,14,15,16,17,18]. Ionization energies of biomolecules are very important because they provide a scale for comparing their oxidative potential in biological reactions [19]. Calculation of the physical properties of biomolecules in the gas phase, such as ionization energy, is important because it is possible to achieve the intrinsic properties of the molecules which may be different from those in solution [20]. The interaction of biomolecules with the bulk and the other molecules and

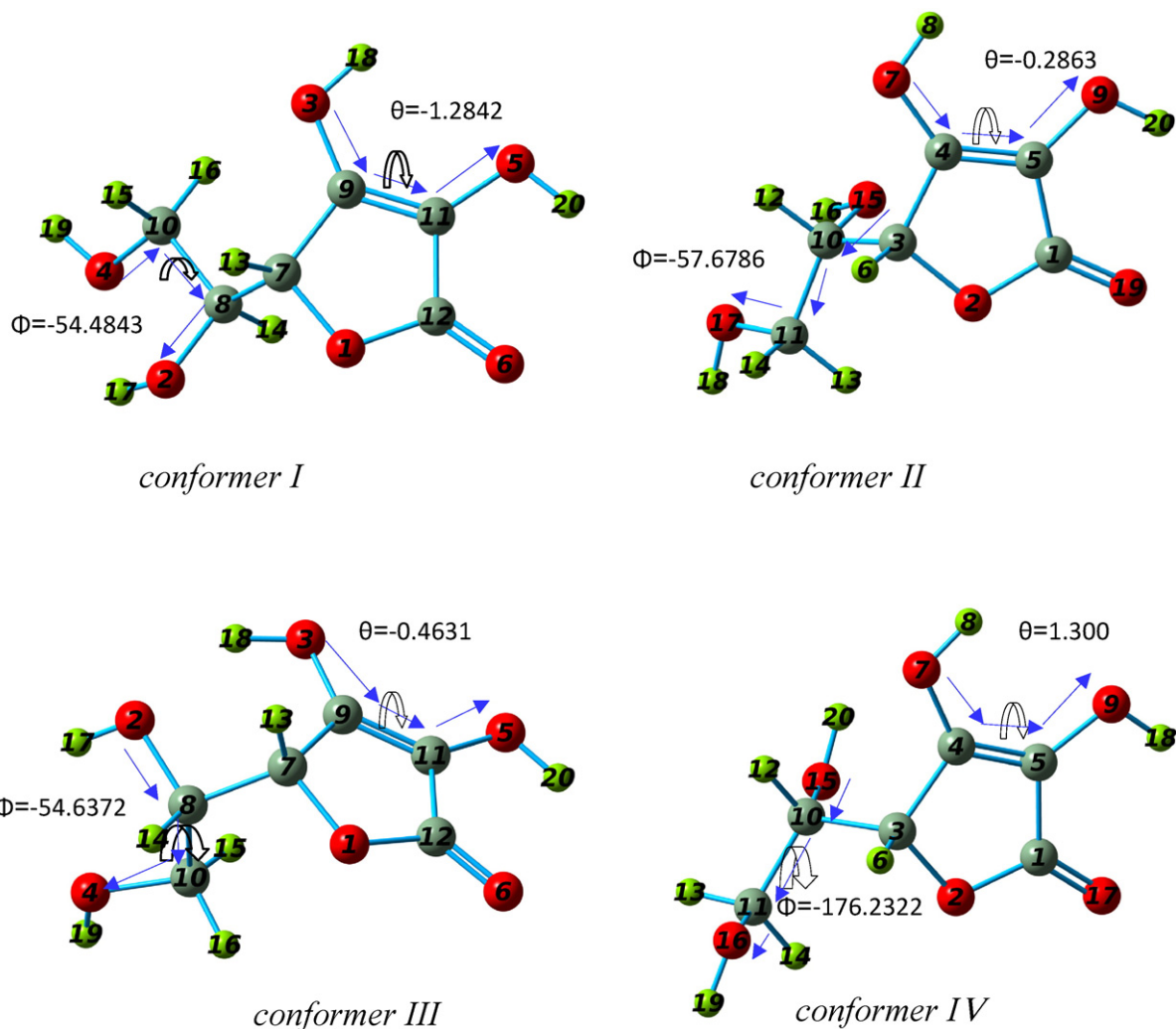
ions present in the biological media changes the electronic structures of biomolecules and produces new chemical properties for them. Ionization energy is the best physical property and excellent guide for exploring how the biomolecule interacts with their surroundings. Comparing the gas phase ionization energy with that in the biological media helps to understand the effect of surrounding on the electronic structure of biomolecule. For example, Nolting et al. [21] determined the photoionization of lysine in the gas phase and aqueous solution at different pH, separately. They found that changing the pH of an aqueous solution of lysine from basic to acidic results in nitrogen 1s and carbon 1s chemical shifts to higher binding energies compared to the gas phase. These shifts were associated with the sequential protonation of the two amino groups, which affects both charge state and hydrogen bonding to the surrounding water molecules.

The advantage of the simulation of the photoelectron spectra of biomolecules in the gas phase is using them as a useful supporting guide for determining the degradation temperature of biomolecules. In this case, comparison of the calculated gas phase photoelectron spectrum of biomolecule with its experimental photoelectron spectrum at different temperatures helps us to determine the temperature of degradation of biomolecule and select the appropriate temperature for evaporation of the sample.

There are a limited numbers of theoretical and experimental published papers on the gas phase ionization of vitamins in literature. Katsumata et al. [22] reported the first experimental He-I photoelectron spectrum of vitamin A in the gas phase. Jericevic et al. [23] recorded the He-I photoelectron spectra of some derivatives of vitamin A including *trans*-retinoic acid, *trans*-retinal, and  $\beta$ -carotene in the gas phase. Novak et al. studied the electronic structures of vitamin D<sub>2</sub> and D<sub>3</sub> using photoelectron spectroscopy technique and found that vitamin D

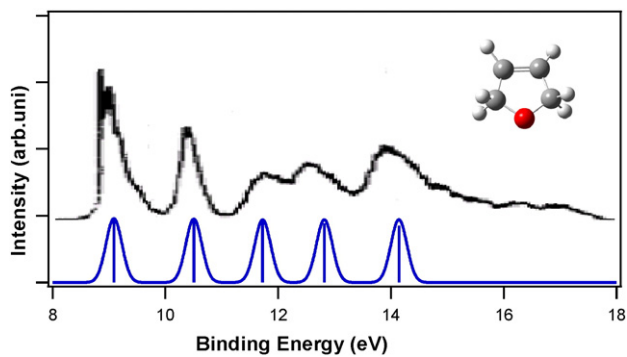
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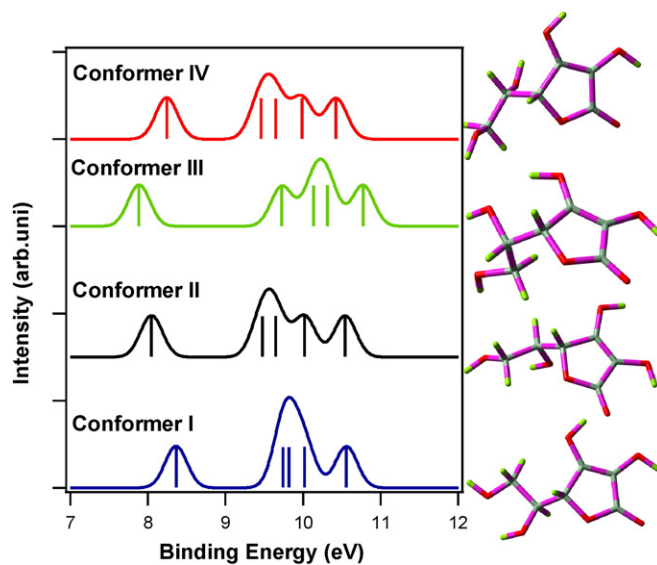


**Fig. 1.** The optimized structures of favorable conformers of vitamin C in the gas phase. The atoms of each structure have been numbered, sequentially. Two dihedral angles have been demonstrated for each conformer by arrows.

has steroid structure due to the similarity of its photoelectron spectrum with the spectra of steroids [24]. Nagaoka et al. recorded the He-I photoelectron spectrum of vitamin E and its derivatives [25]. Recently, Dossmann et al. have performed vacuum ultraviolet photoionization study on vitamins A and B<sub>1</sub> using Aerosol thermo desorption and synchrotron radiation [26]. Lately, Abyar et al. [27] have performed high



**Fig. 2.** Comparison of the calculated photoelectron spectrum of 2,5-Dihydrofuran obtained in this work (blue solid line) with its experimental photoelectron spectrum (black solid line) taken from reference 48. Vertical lines show the calculated position and intensity of ionization bands.



**Fig. 3.** The calculated photoelectron spectra of the conformers of vitamin C shown in Fig. 1. Vertical lines show the calculated position and intensity of ionization bands.

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