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## Computational notes on the effect of solvation on the electronic properties of glycine

Osama Osman, Abdelaziz Mahmoud, Diaa Atta, Aly Okasha and Medhat Ibrahim

Spectroscopy Department, National Research Center, 33 El-Bohouth St. 12311 Dokki, Giza, Egypt

### ABSTRACT

Amino acids are considered as the building units of protein structures. The amino acid glycine was subjected to *ab initio* quantum mechanical calculations at HF/3-21g\*\* level of theory. Glycine is optimized in gas phase then different solvents were applied using Polarizable Continuum Model (PCM) and the integral equation formalism variant (IEFPCM) which is the default SCRF method. The studied solvents are water, acetonitrile, DMSO, nitromethane, methanol, ethanol, acetone, dichloro-methane, dichloro-ethane, chlorobenzene, diethyle ether, toluene, benzene, CCL4 and cyclohexane respectively. Results indicate small geometrical changes in the COOH group as a result of solvation. Total dipole moment indicates an increase in the reactivity of glycine due to the effect of solvation with water. This may be an indication that water is the most favorable solvent for biological molecules such as amino acids and consequently proteins. The calculated HOMO-LUMO band gap energy remains unchanged with changing the type of solvents.

**Keywords:** HF/3-21g\*\*, Glycine, PCM, SCRF and Electronic properties.

### INTRODUCTION

Amino acids are considered as the building units of protein structures. Studying amino acid structures through different spectroscopic tools is considered as the first step towards understanding the molecular structure of proteins. Amino acids could be observed in gas phase in the neutral form, which means that its net charge of the molecule is corresponding to zero [1]. In the aqueous solution and in solid phase, amino acids could perform zwitterionic molecules that enable the formation of hydrogen bonds and stabilize the ionic conformation [2]. The amino acid L-alanine is the smallest naturally occurring chiral amino acid. The assignment of its fundamental vibration is of importance for understanding its activity. Whereas, the crystalline form study helps in the study of a wide range of intermolecular interactions essential for chemistry and biology. On the other hand, low frequency vibrations are important in enzymatic reaction because it contains information on weak reactions [2-3]. Moreover, the amino acid glycine is the simplest protein structure unit [4-5]. Also, it is the smallest and unique non-chiral amino acid that can act as a neuro-inhibitor in mammalian nervous system. The molecule represents non-rigid properties generated by internal rotation and the wagging of amine group [6]. Recently, glycine has been the object of particular attention due to its possible presence in interstellar space and to its use in the design of bio-nano-devices [7]. Among biological molecules the asparagine is an important amino acid that functions in the metabolic control of some nerve cells and brain tissues. Whatever, little work has been done to study the vibrational properties of asparagines [7-9].

Scientists in both chemical and biochemical fields pay their great interest to study the application of hydrogen bonding. It is stated that, hydrogen bonding is omnipresent in nature. It plays a critical role in stabilizing the structures of biological molecules such as proteins or nucleic acid. In view of the role of water in the structural and functional properties of macromolecules and their interactions, considerable attention has been paid to the exploration of the properties of solvated biomolecules [5]. Alanine among other structures was studied by D-Gauss molecular modeling technique [10]. Amide group among other groups were subjected to D-Gauss molecular

modeling to investigate the physical reasons for their functionality [11]. Higher level of theory was followed to analyze the metal interaction with protein [12]. DFT together with FTIR were utilized to investigate the spectral and deconvolution of the natural protein gelatin [13]. Semiempirical calculations were used to investigate the mechanism of Cr interaction with natural protein [14]. Also DFT was used to investigate and analyse the spectroscopic features of organic structures such as [ $\alpha$  (2, 5 dimethylfuryl) ethylidene] (dicyclopropyl methylene) 2, 5 furadione [15]. Recently the functionality of some amino acids could be achieved with the help of molecular modeling to understand biological interactions as well as many other interactions [16-21].

Based upon these considerations modeling study will be directed toward glycine with a special interest to its COOH functional group, total dipole moment and energy band gap. This modeling study will be conducted with ab initio calculations at HF/3-21g\*\* level of theory.

## MATERIALS AND METHODS

### 2. CALCULATION DETAILS

All calculations were carried out with GAUSSIAN03 [22] implemented on personal computer at Spectroscopy Department, National Research Centre.

Glycine is optimized in gas phase, water, acetonitrile, DMSO, nitromethane, methanol, ethanol, acetone, dichloromethane, dichloro-ethane, chlorobenzene, diethyle ether, toluene, benzene, CCL4 and cyclohexane. Each structure is studied with hartree fock level of theory using 3-21g\*\* basis set.

The Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) is the default SCRF method. This method creates the solute cavity via a set of overlapping spheres. It was initially devised by Tomasi and coworkers and Pascual-Ahuir and coworkers [23-25].

Total dipole moment (TDM) is calculated at the same level of theory. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively. The energy difference between the HOMO and LUMO is termed the HOMO–LUMO band gap which is termed  $\Delta E$ . For verification, the vibrational frequencies were calculated in order to ensure that the obtained structures are corresponding to optimized structures.

## RESULTS AND DISCUSSION

The ab initio (HF/3-21g\*\*) optimized structure of the glycine in gas phase is indicated in figure 1. For the effect of solvents Figure 2 presents the ab initio (HF/3-21g\*\*) calculated glycine in solution (S) where S is water; acetonitrile; DMSO; Nitromethane; Methanol; Ethanol; Acetone; Dichloro-Methane; Dichloro-Ethane; Chlorobenzene and Diethyle Ether respectively. The structures of glycine are indicated in symbols and then the surface is indicated with some kind of interest directed towards COOH group. This group is considered the most reactive group in the protein structure.

The effect of solvents upon glycine is indicated in table 1. The table presents the results of bond angle O=C-O, bond distances C=O and C-O, the total dipole moment (TDM) and the energy band gap as HOMO-LUMO difference ( $\Delta E$ ).

Results indicate slight geometrical effect such as an increase in the bond angle which is noticed on going from gas phase to water then slightly decreased to the remaining solvents. The bond distances of COOH has slightly increased ongoing from gas phase to different solvents. It was indicated earlier that the reactivity of a given structure is increased with increasing its total dipole moment and decreasing its band gap energy [11]. Regarding calculated total dipole moment in table 1 it is clear that solvents except CCL4 increases the total dipole moment indicating that glycine is more reactive in solvents. The highest value was recorded with water. Calculated HOMO-LUMO band gap energy shows no indication which remains unchanged with changing the type of solvents.

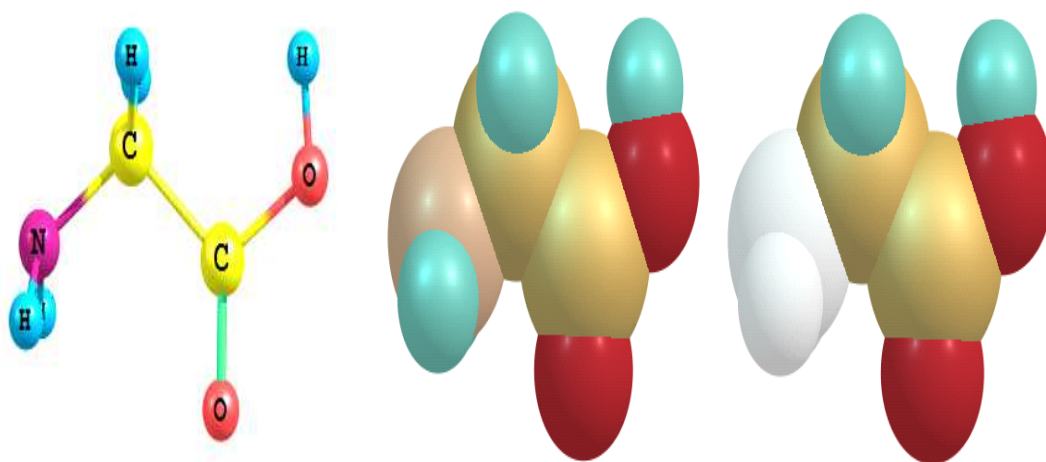


Figure 1. HF/3-21g\*\* Ab initio calculated Glycine in gas phase

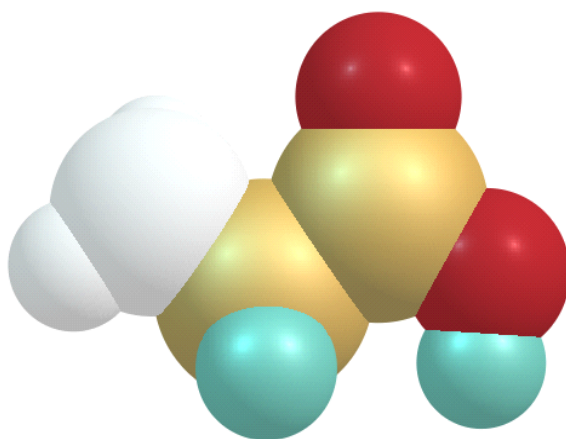


Figure 2. HF/3-21g\*\* Ab initio calculated Glycine in solution (S) where S is water; acetonitrile; DMSO; Nitromethane; Methanol; Ethanol; Acetone; Dichloro-Methane; Dichloro-Ethane; Chlorobenzene and Diethyle Ether respectively

Table1. HF/3-21g\*\* Ab initio calculated bond angle O=C-O (as degree), bond lengths C=O and C-O (as angstrom) respectively, total dipole moment (TDM) as Debye, HOMO-LUMO band gap energy ( $\Delta E$ ) as eV, for glycine in different solvents

Solvent	O=C-O	C=O	C-O	TDM	$\Delta E$
Gas phase	108.687	0.995	0.995	3.471	15.683
Water	109.780	0.999	0.999	6.997	15.645
Acetonitrile	108.767	0.999	0.999	4.506	15.635
DMSO	108.748	0.999	0.999	4.5094	15.638
Nitromethane	108.767	0.999	0.999	4.508	15.635
Methanol	108.744	0.999	0.999	4.501	15.635
Ethanol	108.815	0.999	0.999	4.476	15.635
Acetone	108.744	0.999	0.999	4.456	15.638
Dichloro-Methane	108.738	0.999	0.999	4.345	15.636
Dichloro-Ethane	108.815	0.999	0.999	4.476	15.635
Chlorobenzene	108.751	0.998	0.998	4.229	15.637
Diethyle Ether	108.746	0.998	0.998	4.152	15.639
Toluene	108.738	0.997	0.997	3.920	15.649
Benzene	108.744	0.999	0.999	4.456	15.638
CCL4	108.727	0.997	0.997	3.891	15.652
Cyclohexane	108.727	0.998	0.998	4.192	15.640

## CONCLUSION

Ab initio results at HF/3-21g\*\* level of theory for glycine indicate small geometrical changes in the COOH group as a result of solvation with different solvents. The reactivity is indicated in terms of the calculated total dipole moment and HOMO-LUMO band gap energy. Total dipole moment indicates an increase in the reactivity of glycine due to

the effect of solvation with higher reactivity in case of water. No indications regarding the calculated HOMO-LUMO band gap as it remains unchanged with changing the type of solvents. These results indicate that water among many other solvents is the most favorable for biological molecules such as amino acid and consequently protein.

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