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Analysis of thermo chemistry for some amino acids

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Abstract
Recently density functional theory has gained as great deal of popularity as a tool for quarto chemistry. The present studies that the number and strength of relative hydrogen bonds play central role in detaining reliable proton affinity values.

Keywords: Thermo chemistry and amino acids

Introduction
Natural proteinogenic amino are the building blocks of proteins and peptides which particular in huge number of biological processes. Amino acids are natural in gas phase but have a zwitterionic structure in liquid or in solid phase. The tendency of a molecule to accept a proton (Proton affinity) or to accept an electron (Electron affinity) or to remove an electron (Ionization potential) or the energy different between a molecule and its component atoms (Atomization energy) in the reaction has long been of interest to chemists as they are fundamental to assessing the electron donating and accepting ability and play an important role in electron and proton-transfer process occurring in gas phase of ionized phase. A knowledge of these properties provides important information about the participation of these molecules in transfer reactions and intermolecular forces [1, 2]. Measurement of these fundamental chemical properties of amino acids has become possible with modern mass spectrometric techniques such as (FAB) fast atom bombardment [3, 4], secondary ion mass spectrometry (SIMS) [5] and the soft ion techniques-electrospray ionization (ESI) and matrix assisted laser desorption ionization (MALDI) [1, 6-8], high pressure mass spectrometry [9], fourier transform ion cyclotron resonance (FTICR) mass spectrometry [7] and kinetic methods [3, 8-15] have all been used in evaluating the gas phase properties. Undoubtedly, an accurate experimental determination is the ultimate choice for obtaining these chemical properties even then sophisticated high level ab-initio and DFT calculations have become attractive alternative when the experiment determination is difficult or ambiguous. Therefore, an interplay between theory and experiment becomes very important and crucial for deeper understanding and appreciating the relevance of the observed properties of amino acids together with a knowledge of the limitation of the theoretical methods that have been used to evaluate them. In this study, we have performed calculation of above mentioned thermal propertied if some amino acids with more commonly used ab-initio and density function methods in natural gas phase. The recent literature show that the density functional method (B3LYP) are excellent choice for IP and EA prediction [18-20]. These results have been compared with the available other theoretical calculations and experimental observations.

Computational details: The natural gas phase of amino acids and their corresponding cationic and anionic species were fully optimized employing HF and DFT(B3LYP)/6-31G(d). Zero point correction were performed at the B3LYP/6-31G(d) and B3LYP/6-31G (d, p) energies. Proton affinities were calculated with B3YLP/6-31G(d), B3YLP/6-31+G(d), B3YLP/6-31++G (d, p), B3YLP/6-311+G(d. p) methods. The proton affinities were computed using the following equation:

$$PA(AA) = -\Delta H_{298}$$
$$= -\{[E(AAH^+)-E(AA)] + [H^{corr}(AAH^+)-H^{corr}(AA)]-5/2RT\}$$

where E and H^{corr} are the total energy and enthalpy correction at 298K; AA and AAH^+ denote the amino acid and its protonated form, respectively. The classical estimation of the effect of losing 5/2RT three translation degree of freedom i.e. [(3/2)RT plus the PV term RT]. All the calculations in the present work were carried out at The Department of

Physics, Paliwal (P.G) College, Shikohabad on a Pentium IV PC using G-03W and GAUSS VIEW 4.1 VERSION [17] of ab-initio quantum mechanical program.

Result and Discussion

HF and DFT proton affinity values with a range of basis sets have been computed for some amino acids and presents in table-1. Atomization energy, Electron affinity and lionization potential of the same molecules have been computed using B3LYP/6-31G (d, p) method and presented table-2. It is clear from table-1 that B3LYP in conjunction with 6-311+G(d, p) and6-31++G(d, p) basis set provide the proton affinity values that are in good agreement (difference of ±0.6 Kcal/mol) with the experimental values. However, HF in conjunction with the same basis seta have values very far from the experimental observations which clearly reveals that the electron correlation plays a very important role as far this particular property is concerned. Furthermore, it is also found that in Valine and Leucing the 6-31+G(d) basis set provides good agreement, a difference of ±(0.3 and 0.5 Kcal/mol), respectively, with the experimental results. A very small difference in between our theoretical result and other theoretical methods [16] is probably due to different conformers which should be taken into account in geometrical optimization [15] with the same basis set for PA. The intermolecular hydrogen bonding distance obtained using ab-initio HF and Density Function Theory(B3LYP) methods for all the neutral and protonated amino acids shows not only the relative strength of hydrogen bonds but also shows how the hydrogen bond strength of neutral molecules varies with the protonated molecules [16] which suggests that the number and strength of relative hydrogen bonds play central role in obtaining reliable proton affinity values. The atomization energies are found to be in the order of Leucine> Valine>Serine>Almine>Glycine while for EA and IP the order is Almine>Glicine> Valine>Serine>Leucine and Alanine> Glycine> Leucine> Serine>Valine, respectively. The energy difference between the cation and the neutral molecules is termed as the IP and this is sometimes used as a name for the work needed to remove the top most electrons to infinity from the molecules absorbed onto a surface. However, due to interaction with the surface, this value differs from the IE of the molecules when it is in free space. Therefore, in case of surface absorbed molecules, it is better to use the more general term "Electron Binding Energy". Both these names are also sometimes used to describe the work required to remove an electron from a 'lower' orbital (not the topmost orbital) to infinity, for both the free and absorbed molecules. Therefore, it is essential to specify the orbital from which the electron has been removed. The strength by which the electron is bonded, the greater the ionization energy and is more difficult to remove it. The ionization energy is, thus, an indicator of the reactivity of a molecule with a low I.E. tend to be the reducing agents and to form salts.

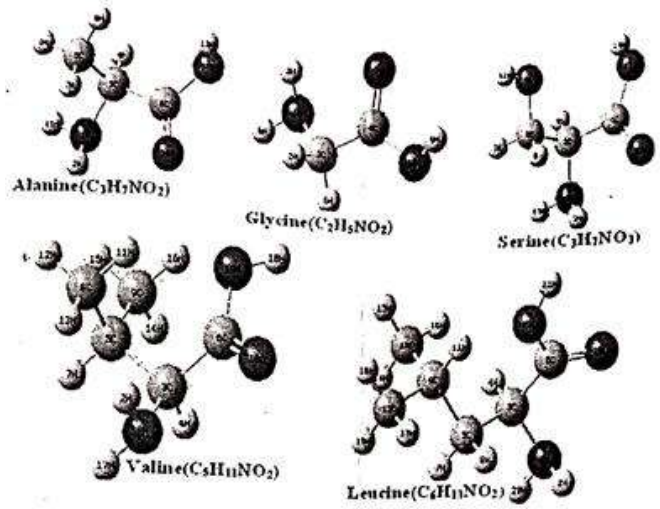

Table 1: HF and DFT Proton affinity of some amino acids in (Kcal/Mol) with different basis sets

	Molecules	Glycine	Alanine	Serine	Valine	Leucine
HF	6-31G(d)[a]	215.8	217.1	220.6	221.4	221.6
	6-31G(d)[b]	214.9	218.9	222.2	221.5	221.6
	6-31+G(d)[a]	215.6	216.8	219.2	220.3	220.2
	6-31++G(d,p)[a]	214.3	214.9	217.1	215.5	216.2
	6-31+G(d,p)[a]	213.3	215.0	217.5	216.3	216.6
	6-311+G(d,p)[b]	213.4	217.4	221.1	220.8	221.6
DFT (B3LYP)						
	6-31G(d)a	215.2	216.9	219.3	220.2	218.9
	6-31G(d)b	216.8	220.8	223.2	223.6	223.8
	6-31+G(d)a	213.5	216.7	218.0	217.3	219.1
	6-31++G(d,p)a	211.6	216.2	218.3	216.9	217.5
	6-311+G(d,p)a	212.1	215.8	218.0	216.3	218.2
	6-311+G(d,p)b	211.5	215.6	217.8	218.9	218.9
Exp.		211.9	215.5	218.6	217.6	218.6

'a' Our present theoretical calculation, 'b' Other theoretical calculation Refs(18), 'c' Experimental values Refs (16)

Table 2: DFT Thermal properties of some amino acids using B3LYP/6-31G(d, p) (in Keal/Mol)

S. No.	Molecules	Atomization energy (AE)	Electron affinity (EA)	Ionization Potential (IP)
1.	Glycine	1181.3619	19.9650	204.7230
2.	Alanine	1501.0969	38.3541	218.7874
3.	Serine	1654.4790	10.4311	197.2952
4.	Valine	2129.2088	18.6980	194.5467
5.	Leucine	2448.4479	3.4393	198.4985

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