SCIENTIFIC REPORT

Dr. Jan URBAN

Short Time Scientific Mission within the COST scientific programme on
Radiation Damage in Biomolecular Systems

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Supervisor: Prof. Dr. Paul SCHEIER

Scientific programme followed the proposed working plan. The calculation of ionization energies at the present state of the theory offers reliable data that can be compare to the experimental results. All up to the present date published theoretical approaches to the study of alanine and glycine [1-7] can be summarized as the using of standard quantum chemical methods with inclusion of correlation (MP2(FC) and CCSD(T)) and density functional methods (B3LYP functional) with the using of basis sets 6-31G* up to the 6-311++G(2df,2pd) quality. The geometrical parameters have been obtained at the MP2 or DFT levels of the theory and energy differences have been calculated by using of CCSD(T) or MP2 methods respectively. Some contributions [8-10] are oriented to the study of the behavior of individual radicals occurring in the process of fragmentation. Our results are based on the calculations performed by using the Gaussian-3 (G3MP2) [11] and G3MP2B3 [12] methods. All calculations have been performed by using of the Gaussian 98 program [13].

Each of molecules, structure and energy of which have been calculated, is given in the Table 1. The energy differences determining the energy necessary for the origin of ions have been evaluated on the basis of the energies calculated for the given molecules. They are presented in the Table 2. It can be seen from experimental results [14,15] that some cations originate at the energy which is below the energy of parent ion. This is probably the case of the ion formation running through the fragmentation of the neutral alanine species following by the ionization of fragments; which means the process of the fragmentation is not always connected with the parent cation.. The formation of COOH+

, NH_2CHCH_2+ and NH_4+ cations are the examples of such a processes. COOH+ cation is formed by the rupture of the C-C bond after which the ionization of COOH radical follows. The formation of $NH_2CHCH_2^+$ cation is energetically favourable via fragmentation of neutral alanine with successive ionization of formed fragment.

We have not finished the calculation of all molecules, it will be done in a short time. Obtained values will be added to the common publication with the experimental data obtained at the departments in Innsbruck and Bratislava.

Our stay in Innsbruck was perfect organized. We had perfect connection to the computer center as well as the approach to the literature, and all resources.

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TABLES

Table1. List of calculated molecules

CH3-CH(NH2)-COOH	NH2=C=CH2(+)
CH3-CH(NH2)-COOH(+)	CH2=N=CH2(+)
NH2-C(CH3)-C(OH)2(+)	CH3-C=NH(+)
NH3-C(CH3)-COOH(+)	OH
CH3-CH-NH2(+)	NH3
CH3-CH-NH2(°)	NH(+)
COOH(°)	NH(°)
COOH(+)	C2H3(+)
NH2-CH-COOH(+)	HCNH(+)
CH3(+)	NH4(+)
CH3(°)	NH(+)
CH2-CH-NH2(+)	CH2NH2(+)
HCOOH neut.	NH2-CH=C=O(+)
CH3-CH-COOH(+)	CH2=C=O(+)
CH2=CH-C(OH)2(+)	CH=CH-COOH(°)
NH2(°)	CH3CH2COOH
NH2-C(CH3)-COOH(+)	CO2(+)
NH2=C=CH2(+)	CO2
	CH3CCCNH2(+)

Table 2. Alanine fragmentation

m/z	ion assignments [1]	ion assignments [2]	AE[1]	AE[2]	our results
89	$NH_2CH_3CHCOOH^+$	the same ion	8.75 $\bar{0}$.05	9.12 $\bar{0}$.2	9.07
74	$NH_2CHCOOH^+$	the same ion	9.3 $\bar{0}$.2	10.74 $\bar{0}$.2	10.07
55	$CH_3C{\equiv}CNH_2^+$	$CH_3C{=}C{=}O^+$	9.3 $\bar{0}$.2	11.34	b
45	$COOH^+$		9.3 $\bar{0}$.2		9.22
44	$NH_2CH_3CH^+$	the same ion	9.05 $\bar{0}$.1	9.10 $\bar{0}$.05	9.51
43	$NH_2CH_2CH^+$		9.05 $\bar{0}$.1		9.41
42	$NH_2CH_2C^+$	$CH_2{=}C{=}O^+$	9.05 $\bar{0}$.1	9.87	11.07[a]
40		$C{=}C{=}O^+$	9.35		
30	$NH_2CH_2^+$		9.05 $\bar{0}$.1		9.57
29	NH_2CH^+		9.05 $\bar{0}$.1		
28	$HCNH^+$	$C{=}O^+$	12.35	10.85,12.8	12.0
27	$C_2H_3^+$		11.5 $\bar{0}$.2		13.28
18	NH_4^+	the same ion	12.0	12.55	10.26
15	CH_3^+	NH^+	12.0	9.4,13.5	

[a] $CH_3C{\equiv}NH^+$ molecule represents the optimal structure

[1] H-W. Jochims et al. Chem. Phys. 298 (2004) 279.
[2] Š. Matejčík results for publication

b- not finished calculation