

QUANTUM-CHEMICAL CALCULATIONS OF THE IONIZATION POTENTIALS OF SOME AMINO ACIDS

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Among high-molecular compounds occupy an important place proteins. Synthesis and study of the properties of polymers, which include both single units of natural amino acids and their sequence, is an important task, which lies at the junction of the chemistry of high-molecular compounds and biological chemistry. Of the amino acids, α -amino acids are the most important - the structural elements of protein substances, which are fragments of polymers. The number of amino acid residues in the peptide chain is very large, so the molecular masses of proteins reach several million. Based on this, the interest in this work was represented by an amino acid, since the capabilities of the machine do not allow the calculation of the whole protein[1].

Modern quantum chemistry is a powerful theoretical tool for computer calculation of the energy of separation of electrons from molecules and atoms and the accuracy of these definitions increases as newer computational technologies appear. If the experimental values of the ionization potentials of molecules are presented in reference books for a limited number of particles, due to the peculiarities of the instrumental methods for their determination, then quantum-chemical calculation methods make it possible to estimate the values of both adiabatic and vertical ionization potentials for almost any molecules and radicals, including for short-lived particles.

Table 1 presents the unrestricted Hartree-Fock (UHF) method using the small orbital basis of 3-21G quantum-chemical software package «Gaussian-2016», the calculated adiabatic and vertical ionization potentials (PI) and electron affinity (EA) for a number of amino acids. Focusing on the magnitudes of the ionization potentials is due to the fact that it is the electron detachment energy that is a measure of the redox properties of any molecule and the relative magnitude of this parameter can be used to judge what role the acid or base will show the substance in the corresponding chemical reaction.

Table 1. The ionization potentials of some amino acids, calculated by the method UHF in basis of 3-21G

AminoAcids	-IP _a , eV	-IP _v , eV	-EA, eV
Histidine	-4,970162952	-6,792904348	-0,246323024
Cysteine	-5,875832736	-8,988831112	-1,885274572
Proline	-6,653361212	-8,14781704	-2,38105
Alanine	-7,296925012	-11,32226011	-2,352994428
Glutamine	-7,437529416	-9,148483916	-2,160687224
Methionine	-7,512335204	-8,273971872	-2,123678904
Glycine	-7,709867112	-8,887085444	-2,486931892
Tryptophan	-	-6,828062252	-2,262187984

A number of the adiabatic ionization potential indicates an increase in the basicity of these compounds. This is also confirmed by electron affinity values. Judging by the negative values of the calculated values of the electron affinity, one can say that the process is endothermic. A dash in Table 1 indicates the fact that the calculations for the indicated parameters for the corresponding molecule fail, since the procedure of quantum chemical optimization of the corresponding ionized structures fixes unstable structural formations.

Reference

1. Barrett G.C., Elmore D.T. Amino Acids and Peptides.—Cambridge: Cambridge University Press, 2004. — P. 13-17.