Leucino ir Izoleucino atpažinimas paremtas fragmentacijos rezultatais electromagnetiniame lauke

Discrimination of leucine and isoleucine via fragmentation by electromagnetic field

Jelena Tamuliene[1], Teodora Kirova[2]
[1]Institute of Theoretical Physics and Astronomy, Vilnius University, Saulėtekio al. 3, LT-10257, Vilnius
[2]Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas iela 3, LV-1004, Riga, Latvia
teo@lu.lv

Proteins are complex molecules essential for many biological functions, such as enzymatic activity and the transport of nutrients and other biochemical compounds across cellular membranes [1]. To determine protein structure, various analytical methods (direct or indirect) are used, and all these methods have their advantages and disadvantages. The determination of the complete amino acid sequence of proteins still remains a challenge, especially for proteins whose residues are leucine (*Leu*) or isoleucine (*Ile*), especially the mass spectrometry-based ones [2]. The composition of *Leu* and *Ile* is identical, thus, distinguishing them by mass is a non-trivial task, because their mass spectra are different only due to the intensity of the m/z 69 peaks, which is dependent on the experimental condition.

We investigated numerically the interaction of *Leu* and *Ile* with dipole electric (DE) and electromagnetic (EM) radiation fields, further conducting a comparative study between the two isomers. Geometry optimization of the *Leu* and *Ile* structures under the action of a DE field was performed, employing the original cc-pVTZ basis with the help of the computational GAUSSIAN09 package [3].

In the case of the EM field, we proceeded using a modified cc-pVTZ basis in which correction coefficients were introduced to the molecular wave functions in order to reflect the elongation of electron orbitals and densities caused by the magnetic field, similar to our recent work [4]. These coefficients were calculated following the procedure of the Anisotropic Gaussian-type orbital method [5, 6]. Since the values of the magnetic field of radiation are very small, (~10^{-5} a.u.) the obtained correction coefficients proved to be independent of the type of atom or orbital.

In the DE and EM fields, *Leu* was partially deformed (Fig. 1 left). In the case of *Ile2* (one of the Ile conformers obtained by us), increasing the field strength leads to the O-H and N -H bond rotations, while in the case of *Ile1*, when the study is performed with the inclusion of both the dipole electric and the corresponding magnetic field, the H transfer is obtained, i.e. the zwitterion form of *Ile1* is formed.

In addition, we have studied the electrostatic potential which also indicates the charge distribution and allows predict different behaviour of *Leu* vs *Ile* in the DE or EM fields, and can be used for these structural isomers' discrimination. For example, for field strength 0.5 a.u. in the case of *Leu*, the fragmentation is field-independent, giving CO_2, C_2H_5N, C_3H_6, and 2H, while *Ile* decomposes into CH_3, C_3H_6, $C_2H_4NO_2$ in the electric dipole field, and into CO_2, C_3H_8N, C_2H_4, H in the electromagnetic field. Moreover, this method could be used for the conformer's (*Ile1* vs *Ile2*) recognition. The latter suggests the relevance of our numerical calculations, which account for corrections to the molecular orbitals due to the magnetic field, and they could be proposed as a possible tool for isomer discrimination.

This abstract is based upon work from COST Action CA18212-Molecular Dynamics in the GAS phase (MD-GAS), supported by COST (European Cooperation in Science and Technology). The numerical calculations with GAUSSIAN09 package were performed at the High Performance Computing Center of Vilnius University "HPC Sauletekis".

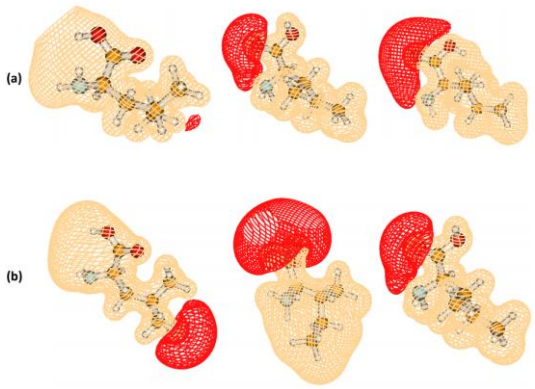

Fig. 1 View of the electric potential of Leu (on the left), Ile1 (in the center), and Ile2 (on the right) obtained with the inclusion of the electric dipole field (a) and along with the corresponding magnetic field (b). The field strength is E=0.40a.u. The contour value is 0.10.

Key words: amino acids, isomers, conformers, basis set, electromagnetic field, fragmentation

References:

[1] G. Wu, F. W. Baser, Z.Dai, D. Li, J. Wang, and W. Zhenlong, Annu. Rev. Anim. Biosci. **2**, 387 (2014).
[2] K. Biemann, Biomed. Environ. Mass Spectrom. **16(1-12)**, 99 (1988).
[3] http://www.gaussian.com
[4] T. Kirova and J. Tamuliene, Materials **16(5)**, 1814 (2023).
[5] P. Schmelcher and L. S. Cederbaum, Phys. Rev. A **37(3)**, 672 (1988).
[6] W. Zhu and S. B. Trickey, J. Chem. Phys. **147**, 2441084 (2017).