NUMERICAL INVESTIGATIONS OF THE IMPACT OF THE MAGNETIC FIELD OF RADIATION ON AMINO ACIDS

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Abstract Amino acids are the structural units of proteins and have important roles as metabolic intermediates in biosynthesis or synthesis of other molecules. Tryptophan is a precursor of the neurotransmitter serotonin, see Savelieva et al. 2008, tyrosine is essential in producing norepinephrine and dopamine, valine and isoleucine are associated with insulin resistance in mammals, see Lynch et al. 2014. After deposition of high-energy ionizing quanta, electrons with different energies are formed and destroy biological molecules, such as DNA and proteins, causing chromosome aberrations, cancer mutations, genetic transformations etc. Structural changes of amino acids are investigated using electron ionization mass spectrometry, while mass spectra are typically interpreted by theoretical calculations, see Tamulienė et al. 2020. We investigate theoretically and numerically the effects of magnetic field of radiation on the fragmentation of different amino acids. The effects are accounted for by using the anisotropic Gaussian type orbitals method, see Schmelcher, et al. 1988, where anisotropy in the wavefunction is used in order to describe the elongation of electron orbitals/densities along the magnetic field direction. As a testing ground for our model we have used light molecules (e.g. H_2), following the procedure outlined by Zhu et al. 2017. Currently, various amino acids are being analyzed, including geometrical parameters of the initial molecule rearrangement. In the case of fragmentation, additional analysis will be performed be in order to determine whether it is due to simple bond cleavage or to more complex reactions involving molecular rearrangements.

References.

Savelieva, K.V. et al.: 2008, *PLoS One*, **3(10)**, e3301.
Lynch, C. J. and Adams, S. H.: 2014, *Nature Reviews. Endocrinology,* **10(12)**, 723.
Tamulienė, J. et al.: 2020, *EPJD*, **74**, 13.
Schmelcher, P. and Cederbaum, L. S.: 1988, *Phys. Rev. A*, **37(3)**, 672.
Zhu, W. and Trickey, S. B.: 2017, *J. Chem. Phys.,* **147**, 244108.