Teoriniai ir skaitmeniniai magnetinio lauko poveikio amino rūgštims tyrimai

Theoretical and numerical studies of the impact of the magnetic field of radiation on amino acids

Teodora Kirova[1] and Jelena Tamulienė[2]
[1]Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, LV-1004, Latvia
[2]Institute of Theoretical Physics and Astronomy, Vilnius University, Sauletekio 3, Vilnius LT-10257, Lithuania
teo@lu.lv

Amino acids are the structural units of the proteins. By joining together, amino acids form peptides (short polymer chains) or polypeptides/proteins (longer polymer chains). The twenty amino acids encoded directly in the universal genetic code are standard/canonical amino acids. Non-protein amino acids also have important roles as metabolic intermediates, such as in biosynthesis or are used to synthesize other molecules. For example, tryptophan is a precursor of the neurotransmitter serotonin [1], serine plays a crutial role in the metabolism and signaling activities in living organisms [2], threonine is an important constituent of collagen, elastin, and enamel protein.

The interaction of molecules with radiation is a fundamental and very important process involved in various fields, e.g. in radiation biology. Shortly after the deposition of high-energy ionizing quanta into a biological medium, electrons with different energies are formed and are able to destroy biological molecules, such as DNA and proteins, and cause chromosome aberrations, leading to cancer, mutations, genetic transformations, etc. [3]. Due to this scientific and medical interest, many research groups have studied the structural changes of amino acids using electron ionization mass spectrometry, where the mass spectra are typically interpreted by theoretical calculations [4].

Motivated by the above, in this work we will investigate theoretically and numerically the effects of the magnetic field of radiation on the fragmentation of amino acids. The radiation field created by a moving change is given by:

$$\mathbf{E}(\mathbf{r},t) = \frac{q}{4\pi\epsilon_0}\left\{\frac{\hat{\mathbf{R}}}{(1-\hat{\mathbf{R}}\cdot\beta)^3 R}\times\frac{1}{c}\left[(\hat{\mathbf{R}}-\beta)\times\dot{\beta}\right]\right\} \tag{1}$$

$$\mathbf{B}(\mathbf{r},t) = \frac{1}{c}\hat{\mathbf{R}}\times\mathbf{E}(\mathbf{r},t), \tag{2}$$

with $\mathbf{E}$, $\mathbf{B}$, and $\hat{\mathbf{R}}$ being mutually perpendicular. During the interaction of matter with the electromagnetic field, the atom/molecule is perturbed by both the electric and the magnetic field. The typical energy shift in the linear Stark effect is $\Delta E_S \sim e\varepsilon a_0 \sim e\varepsilon\hbar/mc\alpha$, while in the Zeeman effect it is $\Delta E_Z \sim eB\hbar/2m \sim e\varepsilon\hbar/2mc$. Since the effects of the electric field on matter are larger by a factor of $1/\alpha$ (α is the fine-structure constant), as a first approximation in our studies we will neglect the terms of the oscillating magnetic field in the Hamiltonian and leave only the ones including the electric field.

The effects of the magnetic field of the radiation will be accounted for only by using the method of anisotropic Gaussian type orbitals (AGTO), first introduced by Schmelcher and Cederbaum [5]. In this basis, the exponential factor of the basis functions has different decay constants along and perpendicular to the direction of the magnetic field. Such an anisotropy gives the flexibility to describe the elongation of electron orbitals and densities along the field direction. In cylindrical coordinates (ρ, z, ϕ), the j^{th} AGTO basis function takes the form:

$$\chi_j(\rho,z,\phi) = N_j\rho^{n_{\rho_j}} z^{n_{z_j}} e^{-\alpha_j\rho^2-\beta_j z^2} e^{im_j\phi}, j = 1,2,3\ldots, \tag{3}$$

where $n_{\rho_j} = |m_j| + 2k_j$, $k_j = 0,1\ldots$ with $m_j = \ldots -2,-1,0,1,2\ldots$ and $n_{z_j} = \pi_{z_j} + 2l_j$, $l_j = 0,1\ldots$, with $\pi_{z_j} = 0,1$.

Eventhough Schmelcher and Cederbaum deduced all the required Hamiltonian matrix elements with respect to such AGTO basis functions, the optimal determination of the sets α_j and β_j was left largely as an open question. Later on, after detailed analysis and extensive numerical exploration, a significant technical advance of the AGTO basis sets was presented by Zhu and Trickey [6].

Following the procedure outlined in [6], we will first use light atoms as a testing ground for our theoretical model. Later on, various amino acids will be analyzed, including geometrical parameters of the initial molecule rearrangement. In the case of fragmentation, additional analysis will be performed in order to determine whether it is due to a simple bond cleavage or to more complex reactions involving molecular rearrangements.

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