Chiral sensitivity in electronic collisions

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The homochirality in living organisms is not well understood and has been extensively discussed in the scientific community since it would be a step forward to understanding the origin of life. Consequently, the aspects of chiral selectivity that led molecules of amino acids and sugars to appear only in, respectively, left-handed and right-handed form which, therefore, defined the helicity of proteins and nucleic acids, still a puzzle nowadays. Molecular handedness is essential for some mechanisms functions in living organisms, such as replication and molecular structure recognition [1]. Thus, several hypotheses for homochirality were proposed. Based on the discovery of the parity non-conservation in weak interactions, Vester and Ulbrich [2] suggested that the left-handed electrons emitted by the β particle decay, or the left-handed radiation emitted by these particles due to their deceleration (Bremsstrahlung) may give rise to the chiral asymmetry selecting enantiomers from the prebiotic molecules. Then, some experiments were performed to test this hypothesis but none of them obtained conclusive results. Campbell and Farago [3] detected electron circular dichroism (ECD) investigating chiral asymmetries through elastic collisions of optically active camphor molecules by polarized low energy electrons. However, Kessler et. al. [4] contradicted it and pointed out ECD only in substituted camphor with heavy atoms of Bromine (Br) and Ytterbium (Yb(hfc3)). Moreover, they identified a possible correlation between transient negative ions (TNIs) and the extrema of transmission asymmetry in substituted camphor. Dreiling et. al. [5] pointed out ECD in 3BrC, 3IC and 10IC, in consistency to the Vester and Ulbrich conjecture, but with relevant discrepancy between 3IC and 10IC. The latter showed unexpected asymmetry amplitude two times bigger than 3IC. Ruivo et. al. [6] estimated the DEA asymmetry through semi-empirical models. They argued that the auto detachment lifetime may be one of the contributions for the remaining factor of ~2 between 3IC and 10IC.

In the present work, the spin-orbit coupling is being implemented through the Distorted Wave Born Approximation (DWBA) in the Schwinger Multichannel Method (SMC) electronic collisions code [7]. In the current stage, only the static-exchange (SE) approximation is already implemented. Then, the integral cross-sections of elastic electron scattering by target molecules of Acid Lactic, Glyceraldehyde, Epichlorohydrin and 2-Butanol were obtained. Asymmetry factors were also calculated for these molecules with the new code and structures near to resonance positions were found in the Acid Lactic and Glyceraldehyde scattering.

References

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