Circular dichroism on condensed amino acids and precursors: results from Time Dependent Density Functional Theory

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The photophysics of interstellar ices and condensed molecules adsorbed on grains is of primary importance in the study of the origin of the specific handedness of the building blocks of life. Here, I present quantum mechanical calculations based on Time-Dependent Density Functional Theory for the absorption and circular dichroism (CD) of isovaline and its chiral precursor 5-ethyl-5-methylhydantoin, observed in meteoritic findings respectively in [1,2] and [3]. The systems are considered in their geometrical conformation as extracted from a full solid (icy) matrix, as a shortcut to understand the behaviour of molecules with fixed orientation, and/or taking into account the full solid matrix. In the context of a possible 'condensation–warming *plus* hydrolysis–recondensation' process, we obtain that: (i) for low-energy excitations, the 'condensed' precursor has a stronger CD with respect to the amino acid, suggesting that the handedness of the latter could be biased by asymmetric photolysis of the precursor in cold environments; (ii) enantiomeric excess could in principle be induced more efficiently in both systems for excitation at higher energies (VUV) [4].

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