Amino acids are small molecules that form the elemental base of peptides and proteins, which are crucial to life. The objective of this work is to identify the normal modes of vibration of the amino acid alanine, \( \text{L-alanine and D-alanine} \). For this purpose, we used the computational chemistry software of the Gaussian09 package, which performs calculations through the Density Functional Theory (DFT), with the B3LYP functional and the base set 6-31 ++ G (d, p); and the polarizable continuum model (PCM). Our calculations using DFT were performed on an isolated molecule in the form zwitterionic of L and D-alanine. The structure initially obtained from the CIF files [1, 2] was optimized for a lower energy conformation and subjected to the frequency calculation. The assignments for each normal mode of vibrational were made with the VEDA4 program [3] (which provides the potential energy distribution for each mode) and the support of molecular visualization software. Thus, the present work intends to contribute to expand the analysis of the normal modes of vibration of the amino acid under study, since the vibration spectra of the amino acid molecules help to obtain information about the molecular conformation and to provide conjectures about the topology of more complex molecules, as well as compare if there are any differences in their L and D forms.

Keywords: Amino Acid. DFT. PED.

References