

The Relationship Study between Topological Indices in Contrast with Thermodynamic Properties of Amino Acids

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Abstract : In this study are computed some thermodynamic properties such as entropy and specific heat capacity, enthalpy, entropy and gibbs free energy in 10 type different Aminoacids using Gaussian software with DFT method and 6-311G basis set. Then some topological indices such as Wiener, shultz are calculated for mentioned molecules. Finally is showed relationship between thermodynamic peoperties and above topological indices and with different curves is represented that there is a good correlation between some of the quantum properties with topological indices of them. The instructive example is directed to the design of the structure-property model for predicting the thermodynamic properties of the amino acids which are discussed here.

Keywords : amino acids, DFT Method, molecular descriptor, thermodynamic properties

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