Abstract:

Piperazine derivatives play a broad range of roles in the field of medicinal and biological effects in living organism specially humans. These effects include a broad scope such as inhibitors of Matrix metalloproteinase, Acetyl CoA carboxylase and neural agents. So, the study of various spatial arrangements of this molecule which can be medicinally effective is the primary objective of the present work. The conformational analysis of ring inversion in two six-membered hexahydropyrimidine derivatives was studied with ab initio quantum mechanical calculations using prevalent computational softwares Gaussian03w and GaussView. The barriers to inversion, the energy gap between various conformers involved in the ring inversion pathways and the influence of two nitrogen atom in the energy and structure of intermediate conformers were studied and interpreted according to the results obtained from these calculations.

Keywords: Conformational analysis, hexahydropyrimidine, ab initio quantum mechanical calculations, anomeric effect

TheUniversity of zabol

Graduate School

The Dissertation of M.Sc.in organic chemistry

Title:

Study of Conformational Changes and the effect of two Nitrogen Atoms on the Energy Barriers and Stereochemistry of hexahydropyrimidine Conformers involved in the Ring Inversion Process

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