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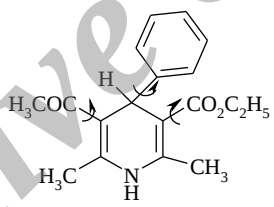
DFT structural studies on the rotamers of ethyl-5-acetyl-4-phenyl-2,6-dimethyl-1,4-dihydropyridine-3-carboxylate

*Seyed Mohamad Sadegh Mousavi, Masumeh Abdoli-Senejania**
Department of Chemistry, Islamic Azad University-Arak Branch, Arak, Iran

E-mail: *mabdoli@iau-arak.ac.ir; abdoli1356@yahoo.com*

1,4-Dihydropyridines (DHPs) are very interesting compounds due to their pharmacological and biological properties [1] Structure-activity studies for some DHPs indicate that the nature and position of the substituents on the DHP ring have very important effect on their biological activities [2]. In view of the importance of the unsymmetrical nature at C_3 and C_5 positions, some new unsymmetrically substituted 1,4-dihydropyridines have been synthesized, in which a carboethoxy group (ester) and acetyl group (keto) are located on the 3- and 5- positions, respectively [3] and investigated conformational analysis of them [4].

1,4-dihydropyridines are flexible molecules, in which the aryl ring and the carbonyl groups can rotate, and the conformation of dihydropyridine ring can change. In the present study we wish to report the theoretical studies on the rotamers and dynamic behaviors of one of new unsymmetrical 1,4-dihydropyridines: ethyl-5-acetyl-4-phenyl-2,6-dimethyl-1,4-dihydropyridine-3-carboxylate. The potential energy surfaces (PES) of ethyl-5-acetyl-4-phenyl-2,6-dimethyl-1,4-dihydropyridine-3-carboxylate have been explored using density functional theory (DFT) B3LYP methods with 6-31G basis set. In addition, the barrier to aryl ring rotation of this compound has been compared with that of the carbonyl groups rotation.



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