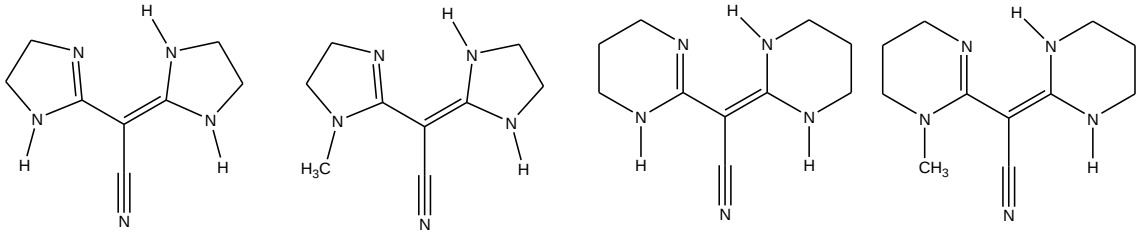
Abstract

The study of rotational barrier around single and/or multiple chemical bonds has been emerged as a significant area of research in organic chemistry. This study, first of all, aids scientists to realize the conformational changes, conformer diversity, their structural stability, reactivity and the factors influencing these subjects. Currently, the effect of chemical compounds conformations on their chemical and biological characteristics has been confirmed. Compounds possessing conjugated double bonds have lower rotational barrier due to the common push-puul effect in comparison to ordinary double bond and the rotation of substituents may occur. So, this rotation would lead to the formation of various conformers. Some derivatives of 2-heterocyclyl-2-ylidene acrylonitrile (heterocyclic ketene aminals or cyclic 1,1-enediamines) (see below) have been prepared recently. In the present work, the rotational barrier of these derivatives around central double bonds has been studied using *ab* initio quantum mechanics calculations and the the governing factors have been revealed.



Keywords :

2-Heterocyclyl-2-ylidene acrylonitrile, Barrier to rotation, Conformational Analysis

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Study of the rotational barrier around enamine carbon-carbon bonds of some 2-heterocyclyl-2-ylidene acrylonitrile derivatives and their conformational analysis using ab initio quantum mechanical calculations

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