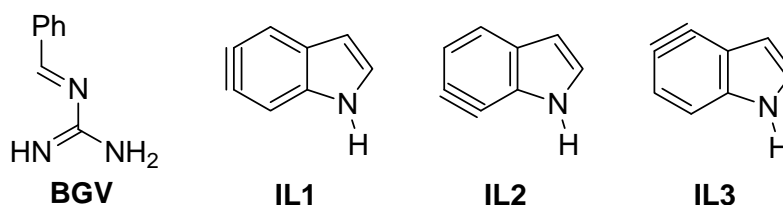


A DFT STUDY OF REGIOSELECTIVITY IN DIELS-ALDER CYCLOADDITION OF *E*-BENZILIDENEGUANIDINE WITH 4,5-, 5,6- AND 6,7- INDOLYNES

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Cyclic guanidines are important subclass of naturally occurring guanidine compounds and medicinal agents [1]. The famous Diels-Alder reaction is very commonly used as a useful approach in the synthesis of cyclic organic compounds in a highly regio and stereoselective manner [2]. Hetero DA reaction, starting from the diaza-diene was shown to produce cyclic guanidines efficiently [3,4]. However, potential of this reaction is still under-investigated.



In this work Diels-Alder cycloaddition of 5,6-, 6,7- and 4,5-indoyline (**IL1-3**) on the *E*-benzilideneguanidine (**BGV**) to produce cyclic guanidinium adducts was studied by DFT approach (B3LYP) prior to experiment. It was shown that the reaction proceeds synchronously without energy barrier in all three cases. The regioselectivity of the reaction is thermodynamically controlled in the case of indoyline **IL2**.

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