

A DFT analysis of the strain-induced regioselective [2+2] cycloaddition of benzyne possessing fused four-membered ring

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The regioselective [2+2] cycloaddition of a substituted benzyne possessing a fused four-membered ring to a ketene acetal has been theoretically studied. This cycloaddition presents a two-step mechanism that is initiated by the nucleophilic attack to the benzyne to give a zwitterionic intermediate. The analysis performed on the basis of the global and local electrophilicity of reagents correctly explain the observed reactivity and regioselectivity in this system. © 2005 Bentham Science Publishers Ltd.