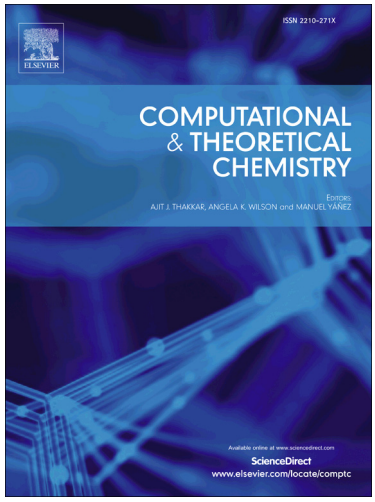

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A theoretical study on [2+2] cycloaddition reactions under visible light irradiation induced by energy transfer

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Abstract

In recent years, [2+2] cycloaddition under visible light has been a hot topic because of low energy consumption and high regio- and stereoselectivities when compared with reactions under UV irradiation. However, the mechanism of [2+2] cycloaddition under visible light irradiation is still unclear. In this research, the visible light catalytic intermolecular [2+2] cycloaddition of 3-ylideneoxindoles has been investigated using density functional theory B3LYP and M06-L methods. The calculated result shows that 3-ylideneoxindoles in triplet excited states can be formed by energy transfer from the triplet excited states of photocatalyst, and then the [2+2] cycloaddition is carried out along the potential energy surface of triplet states. The [2+2] cycloaddition of 3-ylideneoxindoles is more likely to generate head to head products due to the σ–π conjugation. Hydrogen bonds in pre-reaction complex play a key role in the reaction and the strong hydrogen bonding in pre-reaction complex goes against the [2+2] cycloaddition reaction. Furthermore, the electron-withdrawing group of the reactant is beneficial to the reaction because the C=C double bond can be weakened by it.

Keywords: cycloaddition; regioselectivity; visible light; energy transfer; photocatalyst; reaction mechanism