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Theoretical Studies on the Effects of Palmitic Acid Adulteration to the Hydroperoxyl Methyl Linoleate-Tbhq System

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The aim of this research project is to study the effects of adding palmitic acid on the performance of TBHQ(**1**) in inhibiting the autoxidation of vegetable oil. Quantum mechanical software package of Gaussian 09 at the theoretical level of DFT B3LYP/6-31G(d,p) were used to evaluate the physical parameters of TBHQ, hydroperoxyl methyl linoleate radical of C9OO(**2**), palmitic acid(**3**) and their complexes. Based on the stabilization energy of the complex which is comparable to the hydrogen bonding strength, palmitic acid formed more stable complex with C9OO radical than of TBHQ. Details Natural Bond Orbital analyses revealed that the addition of palmitic acid would reduced the effectiveness of TBHQ by weakening the hydrogen bonding (1.910 to 1.963 Å) with the C9OO radical and strengthening the O-H sigma bond of TBHQ (Bond order: 0.673 to 0.683).