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Theoretical Study of the Mechanism of the Oxidation of Linoleic Acid by 1O2

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Abstract : The mechanism of oxidation reaction of linoleic acid C18: 2 (9 cis12) by singlet oxygen 1O2 were theoretically investigated via using quantum chemical methods. We explored the four reaction pathways at PM3, Hartree-Fock HF and, B3LYP functional associated with the base 6-31G (d) level. The results are in favor of the first and the last reaction ways. The transition states were found by QST3 method. Thus the pathways between the transition state structures and their corresponding minima have been identified by the IRC calculations. The thermodynamic study showed that the four ways of oxidation of linoleic acid are spontaneous, exothermic and, the enthalpy values confirm that conjugate hydroperoxydes are the most favorable products.

Keywords : echanism, quantum mechanics, oxidation, linoleic acid H
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