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Simulation Study of Oxidation for Oleic acid by $KMnO_4$ Using Theoretical Calculations

Doaa Muayad, Saadon Abdulla Aowda and *Abbas A-Ali Drea

*Chemistry Department, College of Science, Babylon University, Hilla – Iraq.

Email: aadreab@yahoo.com

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ABSTRACT

Simulation study of oxidation for Oleic acid has been carried out using semi-empirical methods (PM3 and AM1) that are packaged on hyperchem 8.0.9 program. Geometrical properties and vibration spectrums have been calculated. Five different transition states have been suggested and the most probable transition state been investigated depending upon the electronic properties to suggest the most probable pathway of the reaction. The calculations show that first transition state is the most probable than other state due its energetic values of total energy, binding energy, heat of formation, zero pointenergy, and imaginary frequency that's equal to -111016.403, -5670.849, -398.307, 314.119 respectively by kCal mol^{-1} units .The pathway of reaction is spontaneous and exothermic with the change in Gibes energy value and heat of formation value equal to -36122.691 and -110745 respectively

Keywords: semiempirical calculations, transition state, Oleic acid, Dihydroxy stearic acid, oxidation, $KMnO_4$.
