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Novel experimental and three–dimensional (3D) multiphysics computational framework of michaelis–menten kinetics for catalyst processes innovation, characterization and carrier applications

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Oxidation studies of organic substrates alcohols by some inorganic compounds in solution have received considerable attention. Of these, pyridinium fluorochromate (PFC) has long been studied. This complex converts alcohols into aldehyde products smoothly at room temperature and has been claimed that it is a better oxidant than its homologues pyridinium chlorochromate (PCC). Recently, we have synthesized another oxidant i.e. tetramethylammonium fluorochromate (TMAFC), which should be suitable for oxidation of alcohols and has several additional advantages over its homologous pyridinium fluorochromate (PFC) or pyridinium chlorochromate (PCC), e.g. less acidity, selective oxidation under mild condition, better solubility in non–aqueous solvents and so on. Extensive kinetic and mechanistic studies on oxidation of alcohols with chromic acid have revealed that such reactions ordinarily involve a three–electron change, whereby the oxidant, Cr (IV) species, is reduced to Cr (III) [1-212]. In this letter, we report the kinetics of some alcohols oxidation by tetramethylammonium fluorochromate (TMAFC), evaluates the reaction rate constants and temperature dependence on reaction rates. The mechanistic aspects are discussed and a probable mechanism has been proposed. Reaction rates related to temperature was studied and activation parameters were computed. Kinetic parameters such as ΔH^* and ΔS^* were similar in all cases and in two–step mechanism of reaction includes first step (complex formation) is reversible and fast and second step (complex decomposition) is irreversible and slow. Michaelis–Menten kinetics type dependence was pseudo first order in high concentration of alcohol in comprising to oxidant. The reaction was catalyzed by acid and its dependence was unit (Figures 1-3).

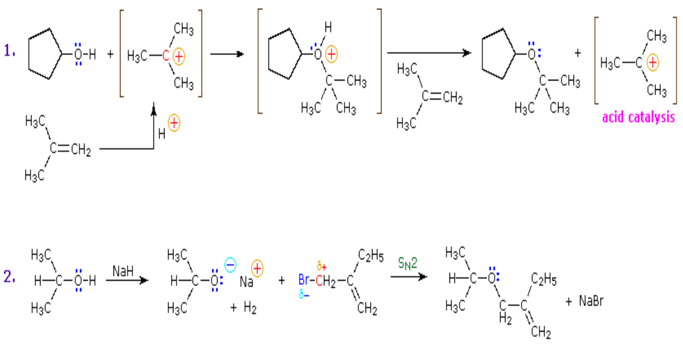

Figure 1. Schematic of the reaction was catalyzed by acid includes two–step mechanism: (1) Complex formation and (2) Complex decomposition

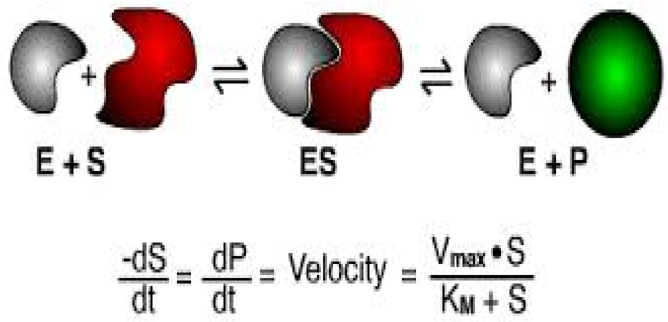

Figure 2. Schematic of Michaelis–Menten kinetics type dependence in high concentration of alcohol in comprising to oxidant

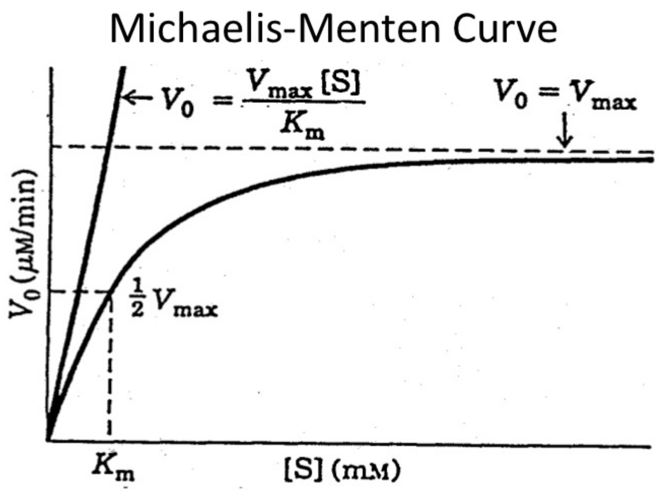

Figure 3. Michaelis–Menten kinetics curve

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