

## RSC Reaction Chemistry & Engineering

### Esterification of propanoic acid with 1,2-propanediol: Catalysis by cesium exchanged heteropoly acid on K-10 clay and kinetic modelling

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#### Supplementary Information

Adsorption of 1,2-PDO (A) on the vacant surface site S is given by



Similarly, adsorption of propanoic acid (B) on the vacant surface site is represented as



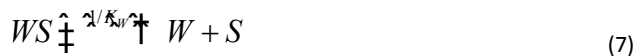
Having adsorbed on surface, reaction of AS with BS on adjacent sites leads to formation of monoester of propionic acid (ES) and water (WS) on the catalytic sites



Second molecule of adsorbed propionic acid (BS) reacts with the adsorbed monoester (ES) on the adjacent site, as follows to give the diester; 1,2-propanedioldipropanoate (FS) and water (WS).



Desorption of product species is given by



Total concentration of the sites,  $C_t$  can be expressed as

$$C_t = C_S + C_{AS} + C_{BS} + C_{ES} + C_{FS} + C_{WS} \quad (8)$$

or

$$C_t = K_A C_A C_S + K_B C_B C_S + K_E C_E C_S + K_F C_F C_S + K_W C_W C_S \quad (9)$$

or, the concentration of vacant sites,

$$C_s = \frac{C_t}{(1 + K_A C_A + K_B C_B + K_E C_E + K_F C_F + K_W C_W)} \quad (10)$$

If the surface reaction (4) is controlling the rate of reaction, then the rate of conversion of A is given by the equation

$$-r_A = -\frac{dC_A}{dt} = k_3 C_{ES} C_{BS} = k_3 K_2 C_{AS} C_{BS}^2 / C_{WS} \quad (11)$$