Supplementary Information

Intrinsic Kinetic Study of 1-Butene Isomerization over Magnesium Oxide Catalyst via Berty Stationary Catalyst Basket Reactor

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Results and Discussion

Table S1: The slope and intercept of linear equations in Figure 10.

	k_1	k_2	K_A	K_B	K_C
m (slope)	-9454.91	-7399.57	1997.88	1614.09	1630.49
C (intercept)	2.203	-0.487	-3.298	-1.297	-1.229

From the Arrhenius's equation as shown in equation 10, this equation was rewritten into the form of the linear equation in equation S1.

$$k_i = A_{0,i} exp\left(\frac{-E_{a,i}}{RT}\right) \tag{10}$$

$$ln(k_i) = \frac{-E_{a,i}}{RT} + ln(A_{0,i}) \tag{S1}$$

Therefore, the slope (m) and intercept (C) for $ln(k_1)$ and $ln(k_2)$ in Figure 10 can be compared with $-E_{a,i}/R$ and $ln(A_{0,i})$ in equation S1, respectively. After that, the activation energies ($E_{a,i}$) and pre-exponential factor according to Arrhenius's equation ($A_{0,i}$) can be calculated from these correlations. For example, the $E_{a,1}$ can be calculated by the slope of $ln(k_1)$, which equals to -9454.9 and gas constant is 8.314 (J/mol/K) as shown in equations S2.

$$m = -9454.9 = \frac{-E_{a,1}}{8.314} \tag{S2}$$

Then:

$$E_{a,1} = 78.608 \text{ kJ /mol} \tag{S3}$$

For pre-exponential factor according to Arrhenius's equation ($A_{0,i}$):

$$C = 2.203 = \ln\left(A_{0,1}\right) \tag{S4}$$

Therefore:

$$A_{0,1} = 9.052 \tag{S5}$$

For deriving the van't Hoff equation, the correlation of adsorption equilibrium constant at different temperatures, T_1 and T_2 were given below.

$$ln(K_1) = \frac{-\Delta H_i}{RT_1} + \frac{\Delta S}{R} \tag{S6}$$

$$ln(K_2) = \frac{-\Delta H_i}{RT_2} + \frac{\Delta S}{R} \tag{S7}$$

Then subtraction yields:

$$ln(K_1) - ln(K_2) = \frac{-\Delta H_i}{R}\left[\frac{1}{T_1} - \frac{1}{T_2}\right]$$

(S8)

which equation S8 is equal to the van't Hoff equation as shown in equation 11. Consequently, the slope (m) and intercept (C) of $ln(K_A)$, $ln(K_B)$, and $ln(K_C)$ in Figure 10 can be also compared with $-\Delta H_i/R$ and $\Delta S/R$ in equation S6 or S7. The adsorption enthalpies (ΔH_i) can be interpreted from the slope of graphs $ln(K_A)$, $ln(K_B)$, and $ln(K_C)$. In case of $ln(K_A)$, the slope of graph is equal to 1997.88, so the ΔH_i can be estimated as shown in equations S9, and S10.

$$K_i = K_{0,i}\,exp\left(\frac{-\Delta H_i}{R}\left[\frac{1}{T} - \frac{1}{T_0}\right]\right)$$

(11)

$$m = 1997.88 = \frac{-\Delta H_A}{8.314}$$

(S9)

$$\Delta H_A = -16.610 \text{ kJ /mol}$$

(S10)

However, the $\Delta S/R$ was not used in van't Hoff equation. For van't Hoff equation, if we know the equilibrium constant at any temperature and the enthalpy, we can determine K at any other temperature. For this research, the reference temperature was fixed at 723.15 K. Therefore, the adsorption coefficients at the reference temperature ($K_{0,i}$) were represented by the adsorption coefficients at 723.15 K. The values of ΔH_i and $K_{0,i}$ were tabulated in Table 4.