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Electronic Supplementary Information

The role of KCl in $FeCl_3 - KCl/Al_2O_3$ catalyst with enhanced catalytic performance for ethane oxychlorination

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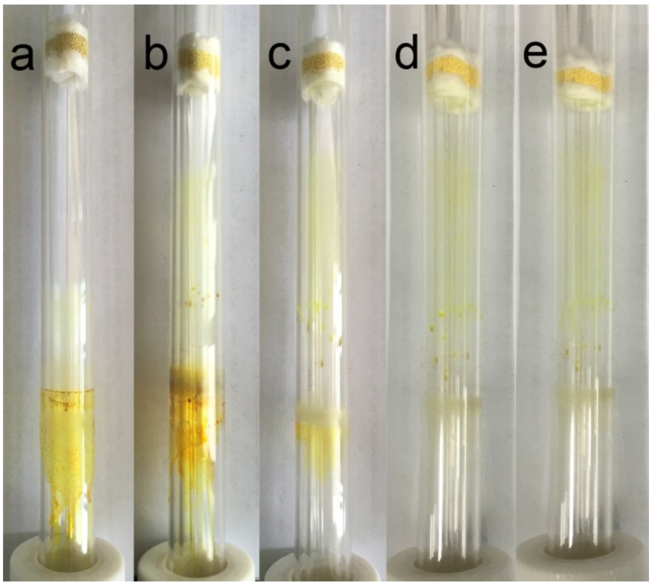

Fig. S1 The loss of active component of the FeKx catalysts after reaction

(a)FeK0(b)FeK0.5(c)FeK1(d)FeK1.5(e)FeK2.

Fig. S1 shows the loss of active component of the catalysts after reaction. The loss is serious in FeK0 catalyst, but is slightly in FeK2 catalyst. This may be because $FeCl_3$ forms a new compound with KCl, which has low vapor pressure, the loss of active component is improved with the addition of KCl.

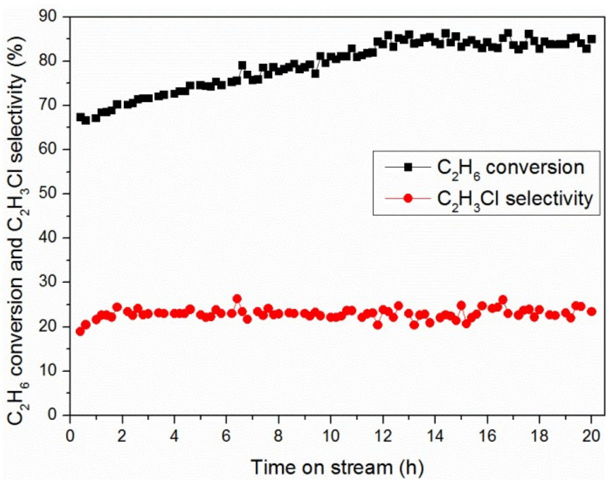

Fig. S2 The C_2H_6 conversion curve and the C_2H_3Cl selectivity curve of FeK0 catalyst for 20h.

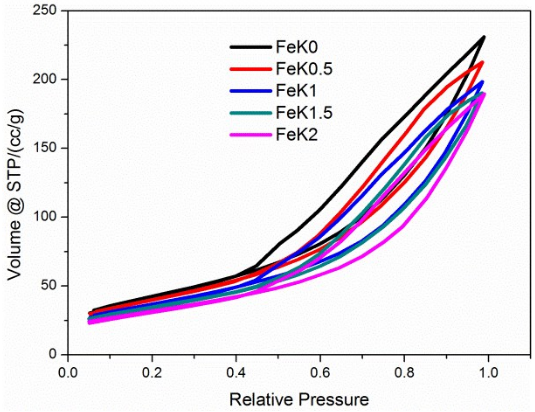

Fig. S3 The N_2 adsorption/desorption isotherms of FeKx catalysts.

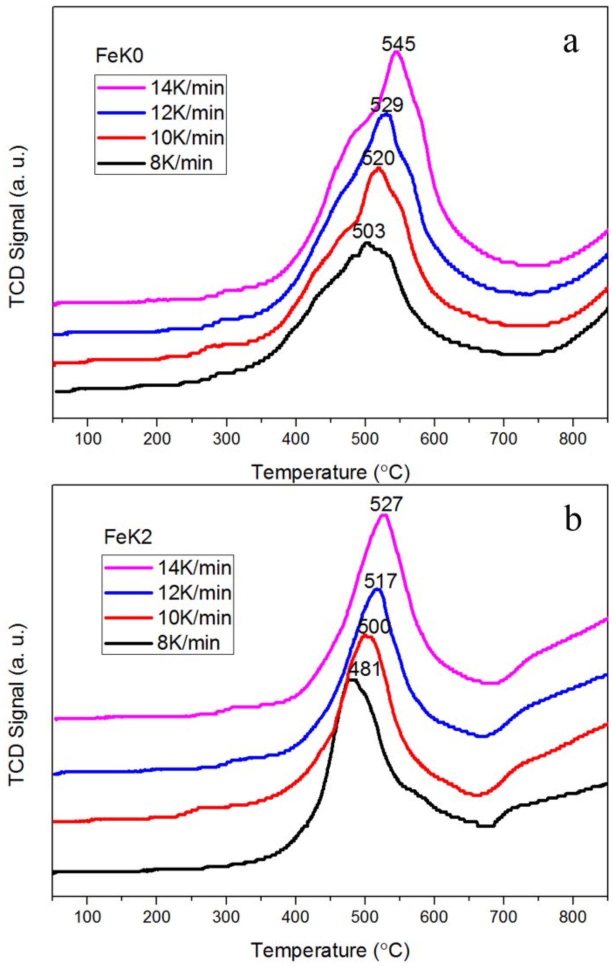

Fig. S4 H_2-TPR curves of FeK0 and FeK2 at different heating rates (β)

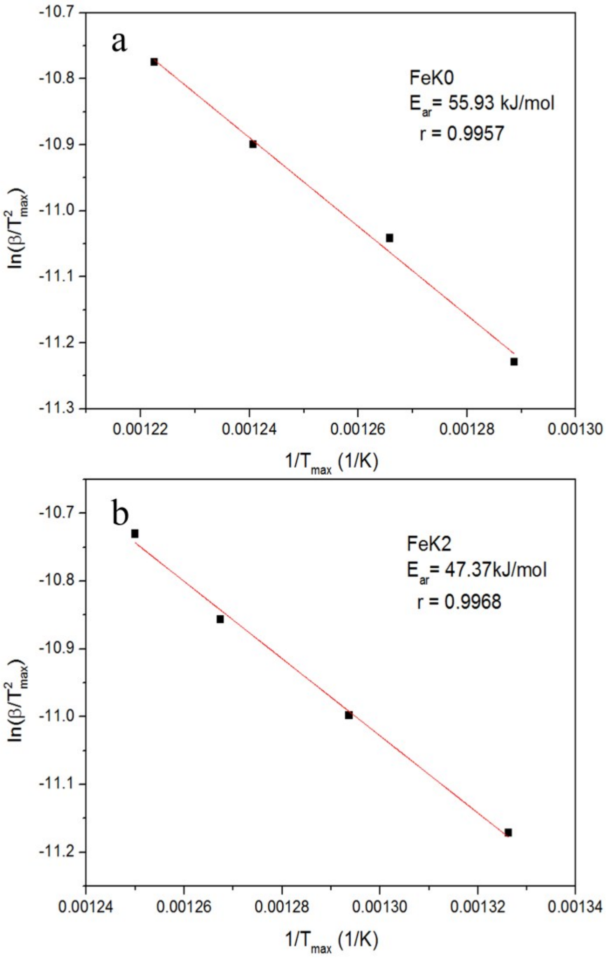

Fig. S5 Kissinger plots for the reduction of FeK0 and FeK2 in 5%H_2/Ar atmosphere.

The apparent activation energy (E_{ar}, here represents reduction activation energy) can be determined by Kissinger method without a precise knowledge of the reaction mechanism, using the equation below:

$$\ln\frac{\beta}{T_{max}^{2}} = \ln\frac{AR}{E_{ar}} + \ln\left[n(1-\alpha_{max})^{n-1}\right] - \frac{E_{ar}}{RT_{max}}$$

Where, β is the heating rate, T_{max} and α_{max} are the absolute temperature and the degree of conversion at the maximum mass-loss rate $(d\alpha/dt)_{max}$, respectively. A is the preexponential factor and n is the reaction order. When n = 1, the term $n(1-\alpha_{max})^{n-1}\approx1$, the equation could be rewritten as:

$$\ln \frac{\beta}{T_{max}^{\ 2}} = \ln \frac{AR}{E_{ar}} - \frac{E_{ar}}{RT_{max}}$$

We plotted a straight line of $\ln(\beta/T^2_{max})$ versus $1/T_{max}$. According to the straight line equation, the preexponential factor A and the reduction activation energy can be calculated from the intercept and slope (E_{ar}/R).