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Abstract

In this paper, the in-situ DRIFTS technology was employed to study the adsorption and reaction behavior of propylene oxide on different substances at different temperatures. And the adsorption behavior of the products at a certain temperature was also studied. The studies shows that the propylene oxide rearrangement involves thermal and catalytic transformation above 200 °C. In the first case, two main reaction pathways are involved: gradual rearrangement to the final products and pyrolysis leading to the formation of different products. In the former situation, the epoxy ring of propylene oxide first adsorbs on the basic lithium phosphate catalyst. Then it forms an intermediate with the bond between C=O and C-O. The intermediate is finally converted to the final products, i.e., allyl alcohol at 300 °C. When the products (propyl aldehyde and acetone) adsorbs on the catalyst, a conjugated structure consisting of basic lithium phosphate and α-H generates.

Keywords: propylene oxide rearrangement, basic lithium phosphate, in-situ DRIFTS technology, intermediate