Supplementary Material

Cyclohexene Epoxidation with H_2O_2 in the Vapor and Liquid Phases over a Vanadium-based Metal-Organic Framework

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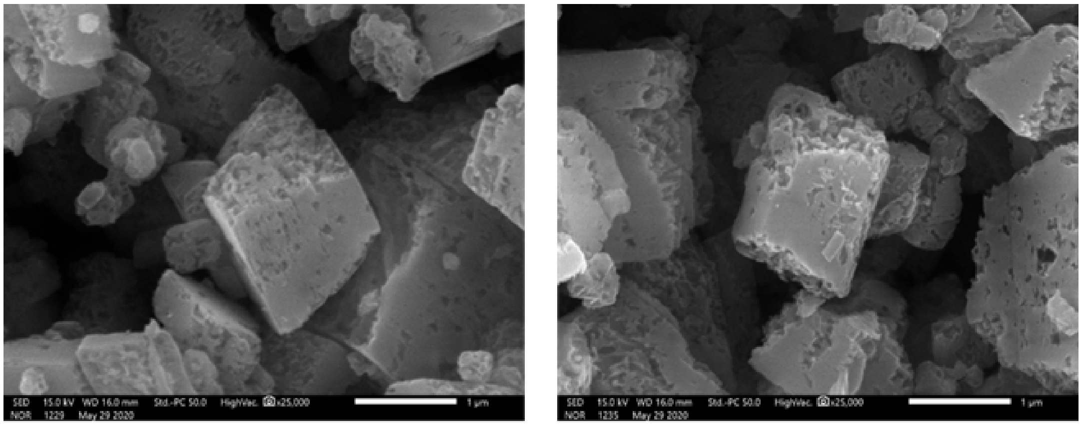

(a) MIL-47(V) before the epoxidation **(b) MIL-47(V) after the epoxidation**

Figure S1. SEM images of MIL-47(V) (a) before and (b) after liquid-phase cyclohexene epoxidation at 65 ℃.

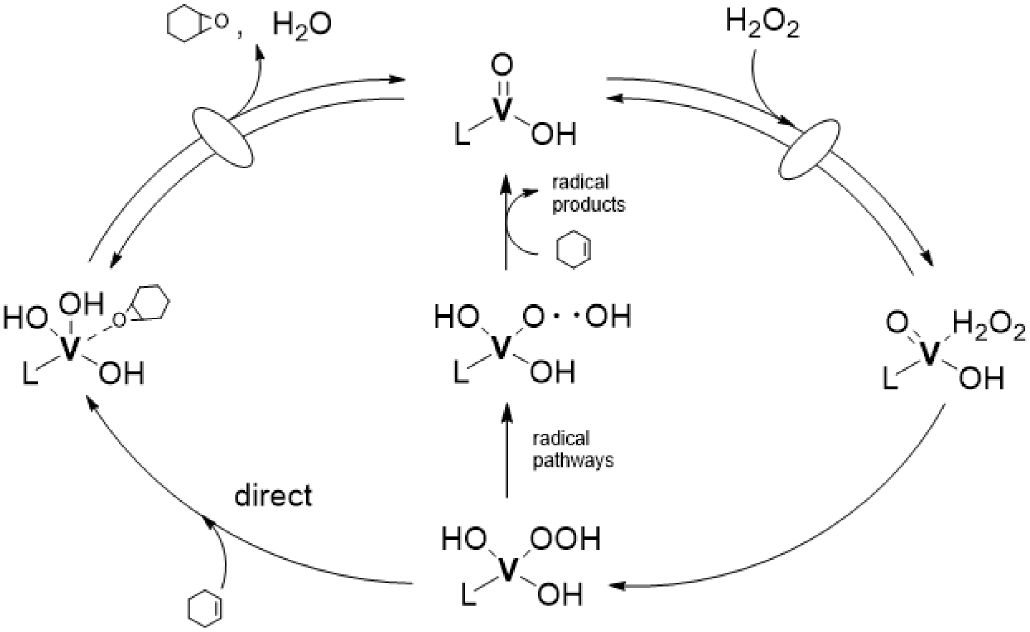

Figure S2. Proposed reaction networks of cyclohexene epoxidation with H_2O_2 over MIL-47(V).

The role of the vanadium node in MIL-47(V) as an active site is proposed. H_2O_2 is first bound to the node, and then forms OOH species. This species can undergo either direct or radical pathways via heterolytic or homolytic cleavage of OOH, respectively. In the former case, cyclohexene is bound to yield epoxide. In the case of radical pathway, cyclohexene reacts with radical and forms cyclohexenyl hydroperoxide, and then yield radical products.