Selective Catalytic Oxidation of Benzene to Phenol by Vanadium Oxide Nanorod (V_{nr}) Catalyst in CH_3CN using $H_2O_{2(aq)}$ and Pyrazine-2-carboxylic acid (PCA)

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Abstract

Vanadium based catalysts were known to be highly efficient for oxidation reactions using O_2 and/or H_2O_2. In this study, we developed a vanadium catalyst that can be prepared by a reaction of VCl_3 in acetonitrile with the addition of 35 wt% hydrogen peroxide (H_2O_2). The catalyst was further characterized by a variety of methods for its material characterization including ^{51}V NMR, XRD, XPS, XAS, EA, ICP-AES, BET, SEM and TEM. Based on the results obtained, the catalyst was identified as vanadium oxide materials (**V_{nr}**) with the morphology and shape of nanorod in dimension of ~40 nm × 450 nm (width × length). The porosity of the materials can be essential for small molecule activation in the heterogeneous surface. This material exhibits exceptional catalytic performance for selective oxidation of benzene to phenol (PhOH) at room temperature using H_2O_2 as oxidant in acetonitrile. The addition of pyrazine-2-carboxylic acid (PCA) as co-catalysts can efficiently enhance the catalytic activity with a percentage selectivity of 87–99% of phenol, and produces *p*-benzoquinone (*p*-BQ) as a minor product. With the deployment of $H_2{}^{18}O_2$, we observed the product phenol to be highly enriched by ^{18}O indicating that the hydroperoxo-vanadium intermediate can be essential for its catalytic conversion. Together with its high NIH shift ratio (80% deuterium remained) observed with the mechanistic probe of 4-$^2H_{0,1}$-toluene, the results suggested the catalytic oxidation reaction mediated by this **V_{nr}** may involve metal based oxygenated intermediates for its highly selective catalytic oxidation of benzene to phenol.

Keywords*: benzene*; *phenol; vanadium oxide nanorod; hydrogen peroxide; catalysis.*