

Supporting information for the paper

In situ Electron Paramagnetic Resonance: A unique tool for analyzing structure-reactivity relationships in heterogeneous catalysis

by Angelika Brückner

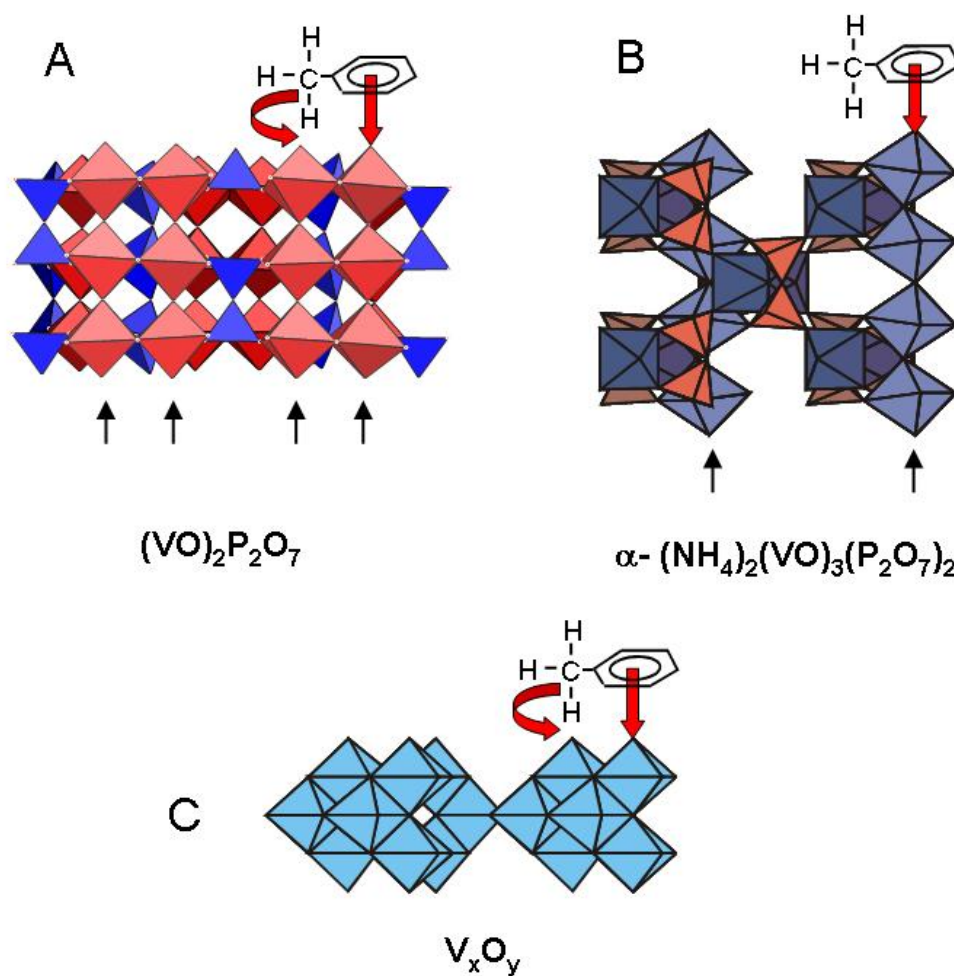


Figure S1. Schematic depiction of the adsorption of the toluene molecule on the structure of $(\text{VO})_2\text{P}_2\text{O}_7$, $\alpha\text{-(NH}_4)_2(\text{VO})_3(\text{P}_2\text{O}_7)_2$ and V_xO_y clusters assuming V_2O_5 structure. The distance of the chains of VO^{2+} octahedra in the crystal structure (marked by arrows) fits the distance between the centre of the aromatic ring and the C-atom of the methyl group only in cases A and C but not in case B. This is assumed as one reason why crystalline $\alpha\text{-(NH}_4)_2(\text{VO})_3(\text{P}_2\text{O}_7)_2$ is catalytically inactive.

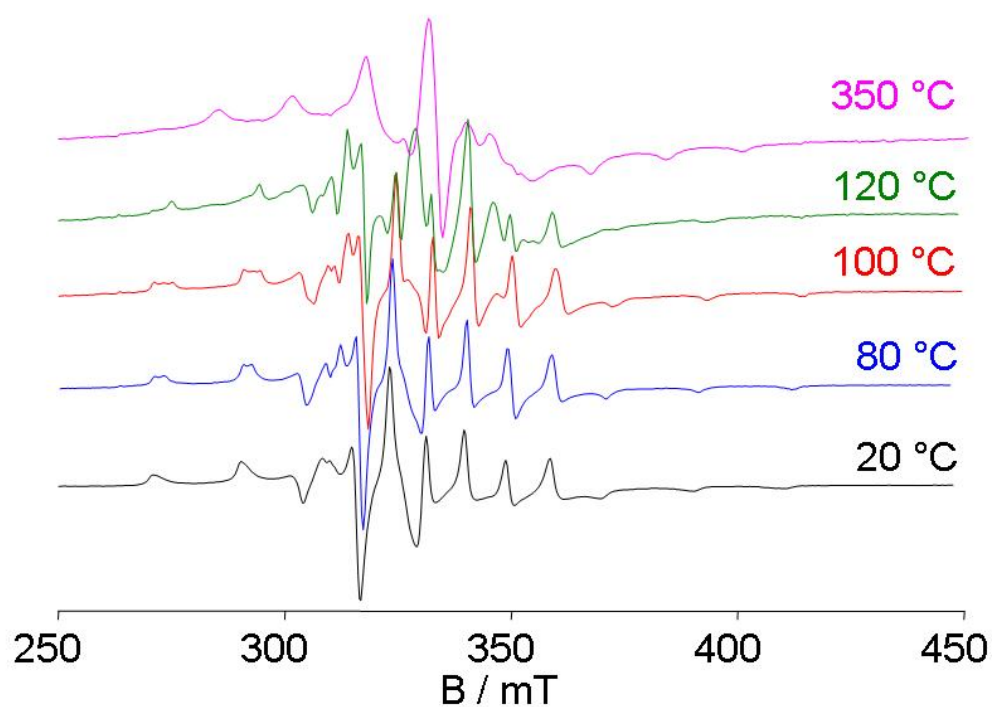


Figure S2. Complete in situ-EPR spectra of $\text{H}_4\text{PVMo}_{11}\text{O}_{40} \cdot x \text{H}_2\text{O}$ during heating in N_2 flow.