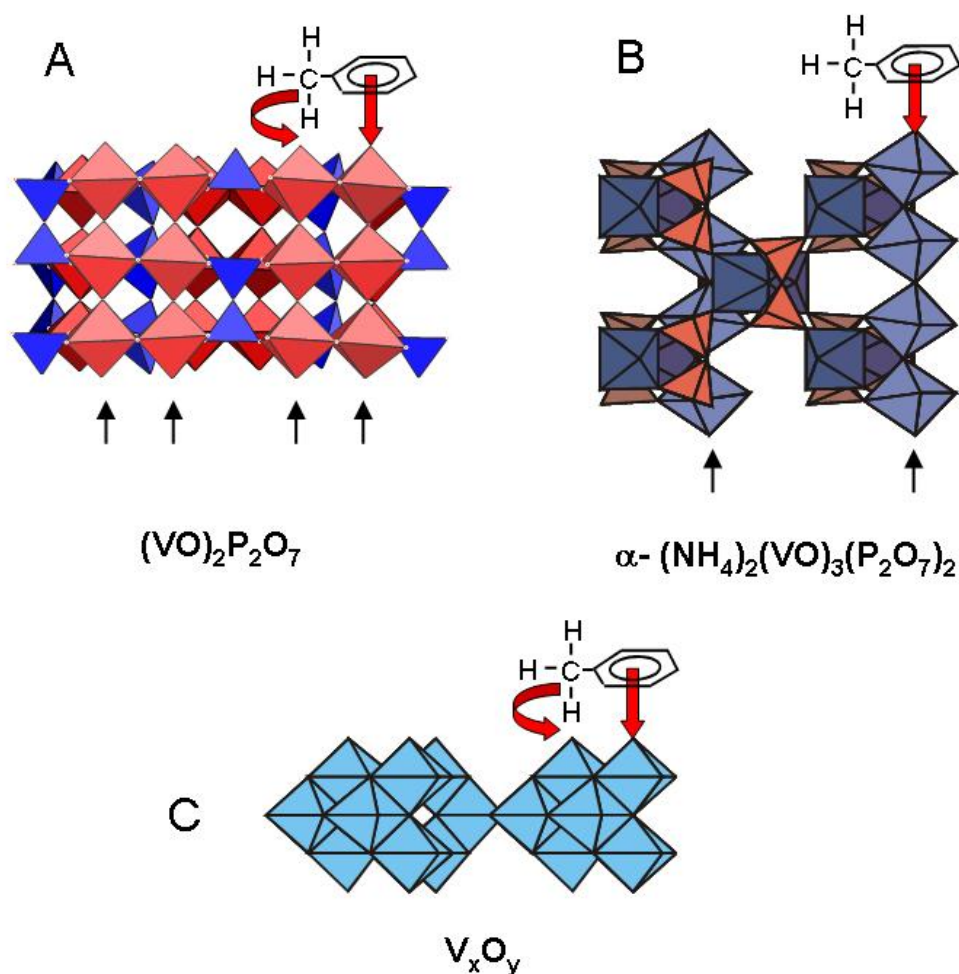


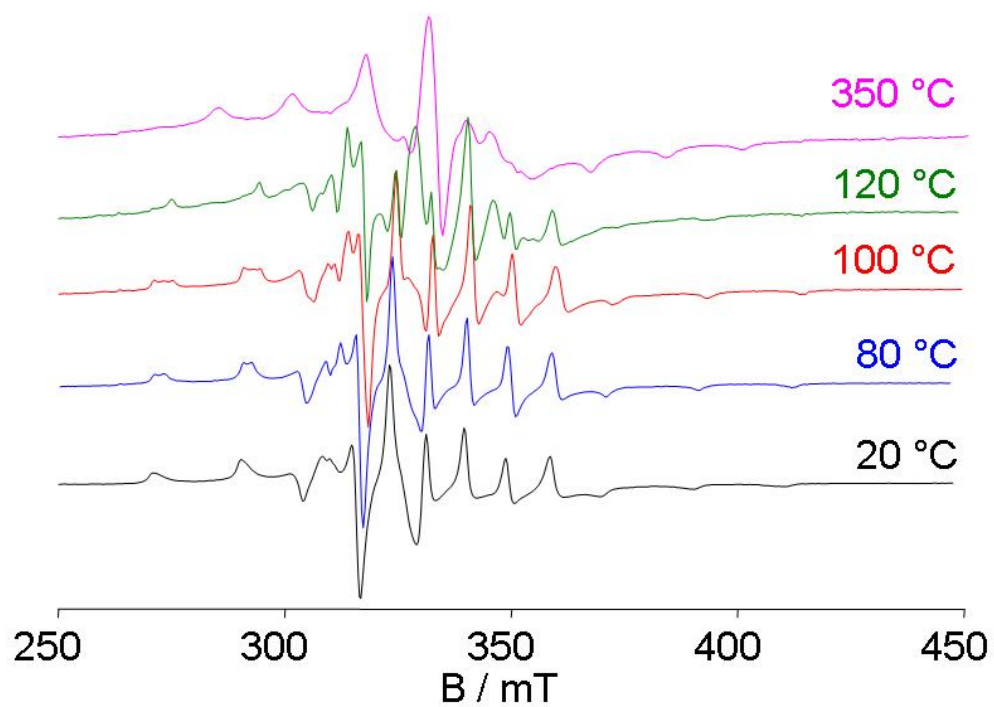
Supporting information for the paper

## 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  $(VO)_2P_2O_7$ ,  $\alpha-(NH_4)_2(VO)_3(P_2O_7)_2$  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  $\alpha-(NH_4)_2(VO)_3(P_2O_7)_2$  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  $\text{N}_2$  flow.