Electronic structure of $\beta$-VOPO$_4$

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Abstract

Vanadium phosphorus oxides are used as catalysts in the selective oxidation of $n$-butane to maleic anhydride. The working catalyst comprises besides the main pyrophosphate phase in which the vanadium is in a 4+ oxidation state also a, predominantly preparation dependent, amount of different pentavalent vanadyl-orthophosphate phases. In order to elucidate the role of the pentavalent phases it is necessary to investigate them in detail. The present work reports the synthesis, characterization and a detailed investigation of the electronic structure of bulk $\beta$-VOPO$_4$ in company with simulated and experimental core-shell excitation spectra.