Supplementary information

Vanadium-based polyoxometalate complex as a new and efficient catalyst for phenol hydroxylation under mild condition

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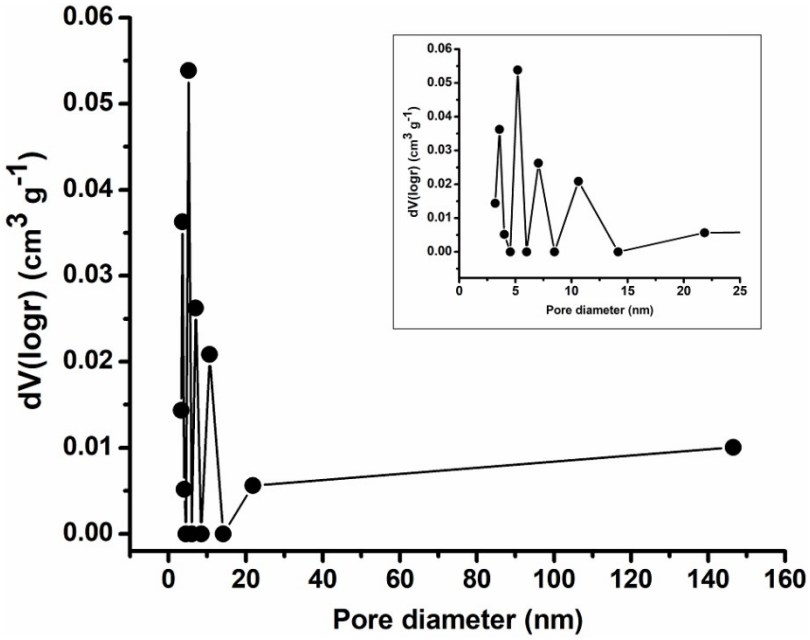

Fig. S1 The pore size distribution curve for compound **1**

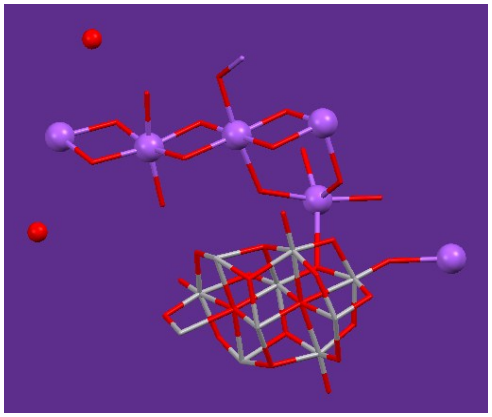

Fig. S2 The molecules in the assymmetric unit. Colour scheme: O, red; V, grey; Na, purple.

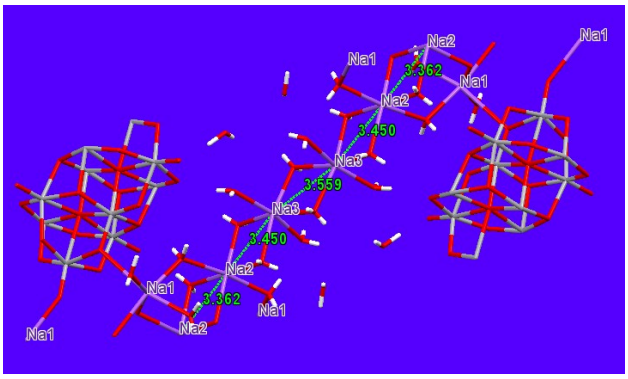

Fig. S3 Polymeric chain showing Na…Na distances. Colour scheme: O, red; V, grey; Na, purple.

Text S4: Determination of H_2O_2 efficiency or effective use of H_2O_2 in the hydroxylation reaction

The calculations are shown with oxidation of Phenol to catechol and hydroquinone as a representative example.

H_2O_2 efficiency (%) = 100 × [mole of H_2O_2 consumed in the formation of Catechol and Phenol products / mole of H_2O_2 converted]

(a) Assuming that one mole of oxidant reacts with one mole of substrate, H_2O_2 (mole) consumed in the formation of di-hydroxyl products (yield: 53 %) from 5 mmol Phenol = 2.65 mmol.

(b) The catalyst was precipitated out during the work up process with ethyl acetate. The product was extracted and the remaining aqueous part containing the precipitated catalyst was separated and the left H_2O_2 was estimated by titration with standard thio solution. The value was found to be: 16.38 mmol.

Since 20 mmol H_2O_2 has been originally used for the reaction,

Therefore, total mole of H_2O_2 converted = (20.0 – 16.38) mmol = 3.62 mmol

Thus, **H_2O_2 efficiency = 100 × [2.65 / 3.62]**

= 73.20 %

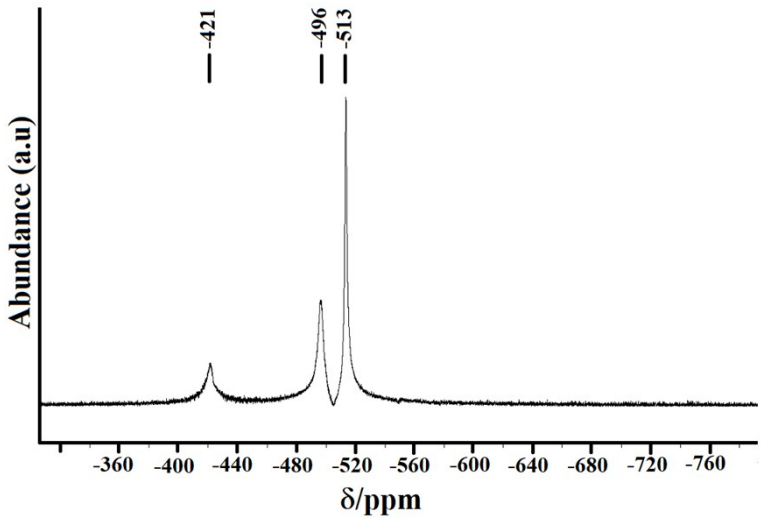

Fig. S5 ^{51}V-NMR spectrum of catalyst **1** after 3rd reaction cycle.

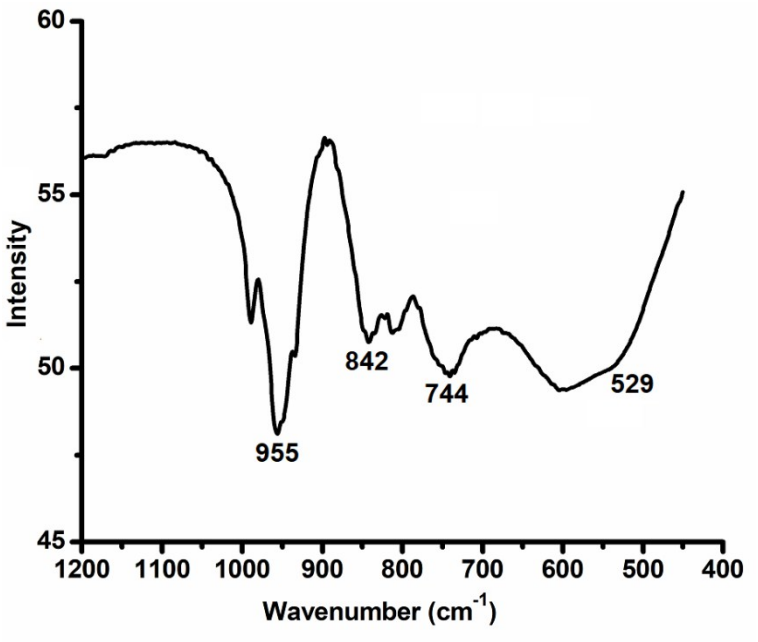

Fig. S6 FT-IR spectrum of catalyst **1** after 3rd reaction cycle