# Oxovanadium(IV) catalysed oxidation of dibenzothiophene and 4,6-dimethyldibenzothiophene

Adeniyi S. Ogunlaja, <sup>*a*</sup> Wadzanai Chidawanyika, <sup>*a*</sup> Edith Antunes, <sup>*b*</sup> Manuel A. Fernandes, <sup>*a*</sup> Tebello Nyokong, <sup>*a*</sup> Nelson Torto, <sup>*a*</sup> Zenixole R. Tshentu<sup>*a*\*</sup>

# SUPPLIMENTARY DATA

#### 1. **AFM and SEM data**





Fig S1. AFM images of p[sal-AHBPD] ,where A1-D1 represents the first to fourth runs.



Electronic Supplementary Material (ESI) for Dalton Transactions This journal is O The Royal Society of Chemistry 2012



Fig S2. AFM images of p[V<sup>IV</sup>O(sal-AHBPD)] where A2-D2 represents the first to fourth runs









**Fig S3.** AFM images of  $p[V^{IV}O(sal-AHBPD)]$  after use, where A3-D3 represents the first to fourth runs

## Table S1. AFM image parameter of the polymer beads

Sample	Size	Avg Roughness	Avg. Mean Height
		(Ra/nm)	( <b>nm</b> )
p[ (sal-AHBPD)]	2x2 micron	4.18	21.31
p[V <sup>IV</sup> O(sal-AHBPD)]	2x2 micron	1.29	8.63
p[V <sup>IV</sup> O(sal-AHBPD)]	2x2 micron	20.57	58.66
after use			

NB: an average of four measurements for each bead was reported.



**Fig S4.** Enlarged SEM images of (A) chloromethylated polystyrene beads, (B) ligand-anchored beads and (C) vanadium incorporated beads  $p[V^{IV}O(sal-AHBPD)]$ .

#### 2. NMR spectra for the intermediates of the catalyst host ligand



Fig S5. N,N-bis(o-hydroxybenzaldehyde)phenylenediamine (sal-HBPD) Schiff base



Fig S6. N,N-bis(4-nitroso-o-hydroxybenzaldehyde)phenylenediamine (sal-NHBPD)



Fig S7. N,N-bis(4-amino-o-hydroxybenzaldehyde)phenylenediamine (sal-AHBPD) Schiff base.

### 3. Isolation and <sup>1</sup>H NMR characterization of the oxidation products

Precipitates (sulfur oxides) were formed after the oxidation process has been completed. These precipitates were collected by filtration and then dried for further analysis. The products were found to be soluble in DMSO, and the <sup>1</sup>H NMR of the product was run without purification (Fig S8-S10).

Due to the insolubility of 4,6-DMDBT in *d*<sub>6</sub>-DMSO, <sup>1</sup>H NMR of 4,6-DMDBT was not carried out.



**Fig S8.** <sup>1</sup>H NMR spectra of dibenzothiophene (DBT)



**Fig S9.** <sup>1</sup>H NMR spectra of dibenzothiophene sulfone (DBTO<sub>2</sub>)



**Fig S10.** <sup>1</sup>H NMR spectra of 4,6-dimethyldibenzothiophene sulfone (4,6-DMDBTO<sub>2</sub>)



# 4. BET Surface area and porosity

Fig S11. Nitrogen adsorption-desorption isotherms for p[sal-AHBPD]



**Fig S12**. Nitrogen adsorption-desorption isotherms for p  $[V^{IV}O(sal-AHBPD)]$