

Supplementary materials

Novel vanadium (III) complexes with rigid phenylpolyboxylate ligands: synthesis, structures and application in C-H bond activation

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Table S1 Characteristic IR bands (cm^{-1}) for the complexes **1** and **2**.

Complexes	1	2
$\nu(\text{O-H})$	3292, 3467	3257, 3439
$\nu(=\text{C-H})$	3056, 3075	3060
$\nu_{\text{as}}(\text{COO}^-)$	1652	1672
$\nu_{\text{s}}(\text{COO}^-)$	1395	1379
$\nu(\text{V-OH}_2\text{O})$	512	539
$\nu(\text{V-Ocarboxyl})$	475	491
$\nu(\text{V-N})$	449	455

Table S2 Characteristic UV-Vis bands (nm) for the complexes **1** and **2**

Complexes	$\pi-\pi^*$ transition	LMCT	d-d transition
1	262	420	742, 1040
2	268	456	742, 1100

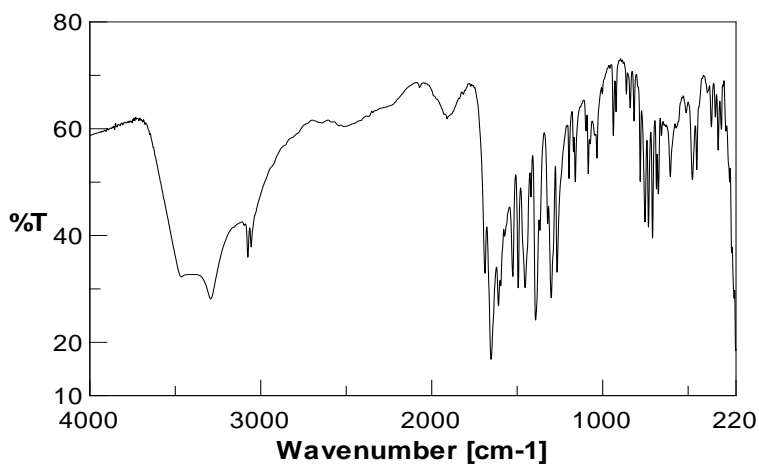


Fig. S1 The IR spectra of the complex **1**

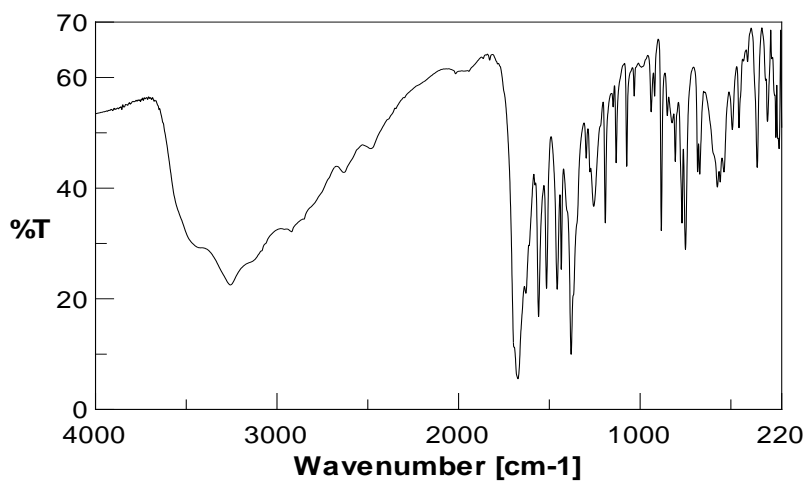


Fig. S2 The IR spectra of the complex **2**

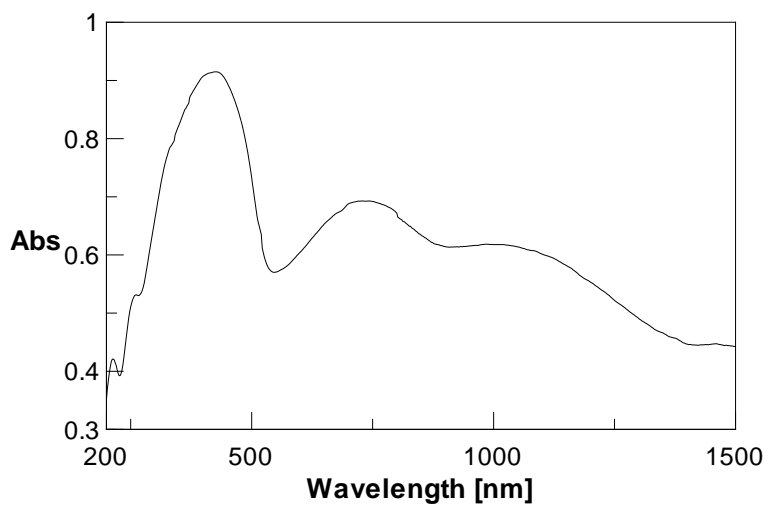


Fig. S3 The UV-Vis spectra for the complex 1

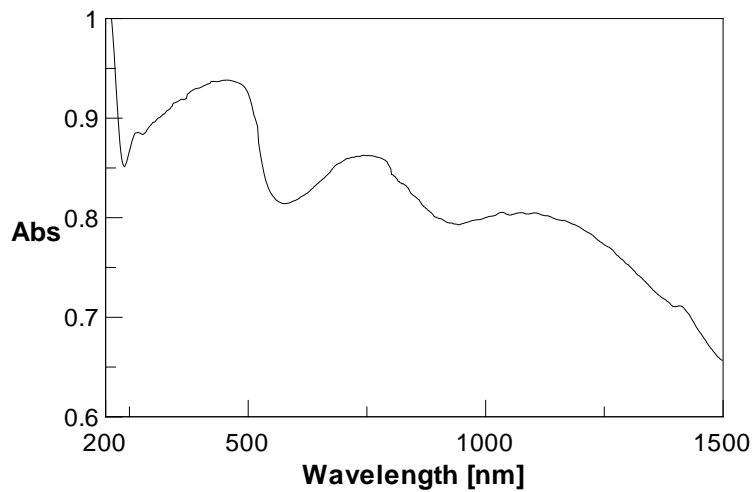


Fig. S4 The UV-Vis spectra for the complex 2

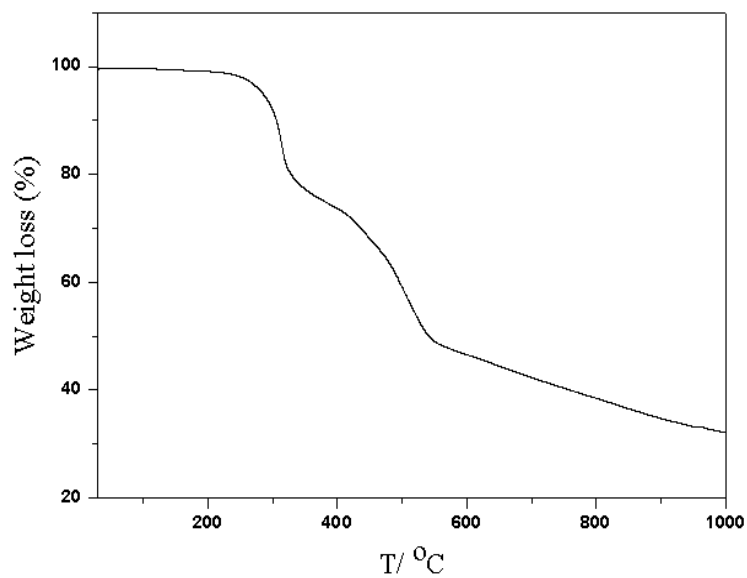


Fig. S5 TG curve of the complex 1.

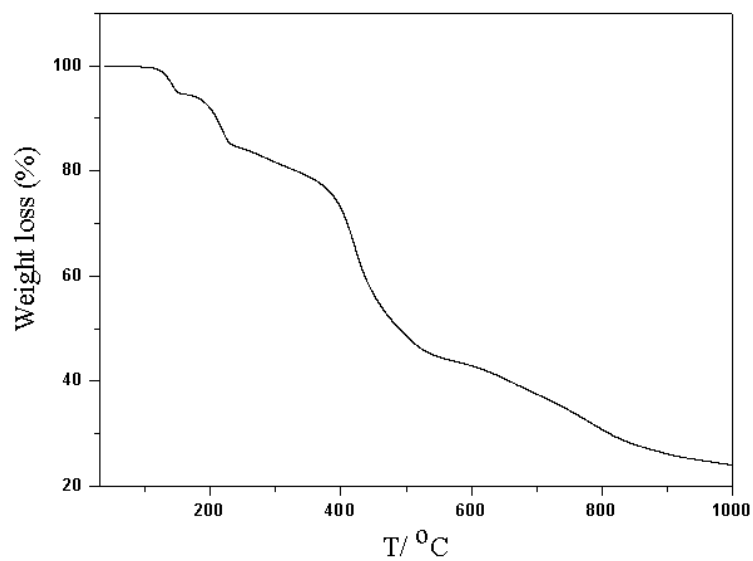


Fig. S6 TG curve of the complex 2.

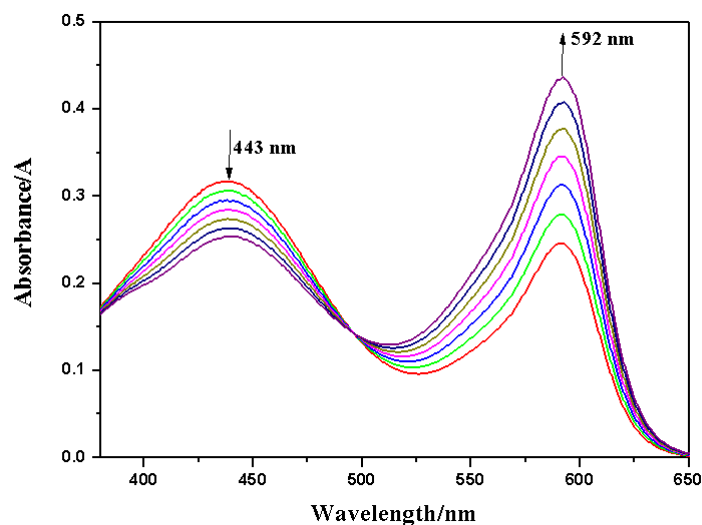


Fig. S7 Oxidative bromination of phenol red catalyzed by the complex **1**. Spectral changes at 10 min intervals, $c(\text{phosphate buffer}) = 50 \text{ mmol/L}$, $\text{pH} = 5.8$, $c(\text{KBr}) = 0.4 \text{ mol/L}$, $c(\text{phenol red}) = 10^{-4} \text{ mol/L}$.

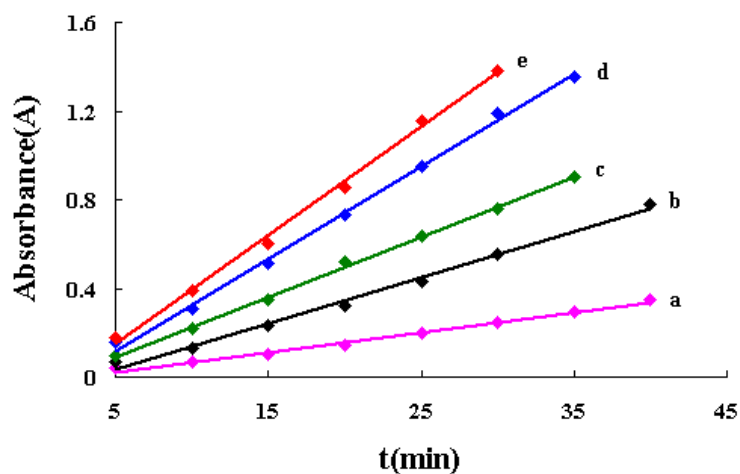


Fig. S8 The measurable absorbance dependence of time for the complex **1**. Conditions used: $\text{pH} = 5.8$, $c(\text{KBr}) = 0.4 \text{ mol/L}$, $c(\text{H}_2\text{O}_2) = 1 \text{ mmol/L}$, $c(\text{phenol red}) = 10^{-4} \text{ mol/L}$. $c(\text{complex } \mathbf{1}/\text{mmol/L}) = \text{a: } 2.3011 \times 10^{-5}$; $\text{b: } 4.602 \times 10^{-5}$; $\text{c: } 6.9032 \times 10^{-5}$; $\text{d: } 9.2042 \times 10^{-5}$; $\text{e: } 1.1505 \times 10^{-4}$.

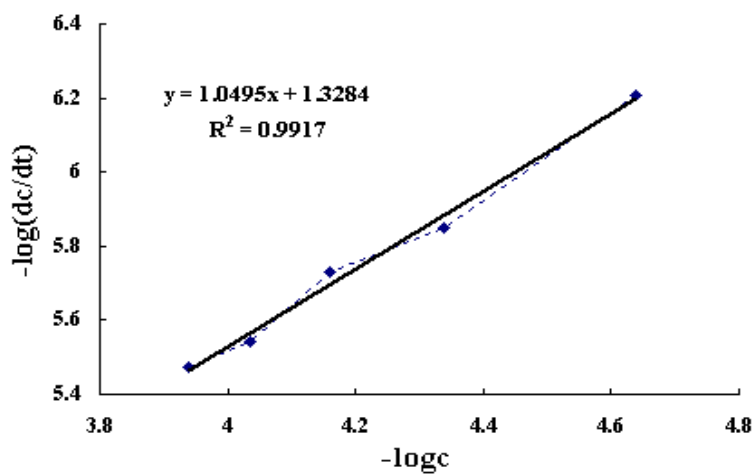


Fig. S9 $-\log(dC/dt)$ dependence of $-\log c$ for complex **1** in DMF–H₂O at 30 ± 0.5 °C (c is the concentration of the oxidovanadium complex **1**; Conditions used: $c(\text{phosphate buffer}) = 50$ mmol/L, $\text{pH} = 5.8$, $c(\text{KBr}) = 0.4$ mol/L, $c(\text{phenol red}) = 10^{-4}$ mol/L).