Supporting Information for

Mimicking vanadium haloperoxidases: vanadium(III)-carboxylic acid complexes and their application in H_2O_2 detection

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Table S1. Selected bond lengths (Å) and angles (°) for the complexes **1**-**2**.

Complex **1**			
V-N(1)	2.123(3)	V-O(1)	2.068(3)
V-O(3)	2.056(3)	V-O(5)	2.139(3)
V-O(6)	2.106(3)	V-O(9)	2.070(3)
V-O(10)	2.076(3)	O(9)-V-O(10)	177.10(11)
O(9)-V-N(1)	92.12(12)	O(10)-V-N(1)	90.09(12)
O(9)-V-O(1)	91.52(11)	O(10)-V-O(1)	87.33(11)
O(9)-V-O(3)	89.39(11)	O(10)-V-O(3)	93.06(12)
O(9)-V-O(5)	86.82(11)	O(10)-V-O(5)	90.34(12)
O(9)-V-O(6)	89.91(12)	O(10)-V-O(6)	89.23(12)
N(1)-V-O(1)	72.99(12)	O(1)-V(1)-O(3)	146.18(11)
N(1)-V-O(3)	73.20(12)	O(1)-V(1)-O(5)	78.12(11)
N(1)-V-O(5)	151.05(12)	O(1)-V(1)-O(6)	139.13(11)
N(1)-V-O(6)	147.77(12)	O(3)-V(1)-O(5)	135.66(11)
O(5)-V(1)-O(6)	61.18(11)	O(3)-V(1)-O(6)	74.66(11)
Complex **2**			
V-N(1)	2.1050(17)	V-O(1)	2.0973(15)
V-O(1W)	2.0339(15)	V-O(2)	2.1201(16)
V-O(2W)	2.0527(15)	V-O(5)	2.0569(14)
V-O(7)	2.0461(14)	O(1W)-V-O(2W)	178.69(7)
O(1W)-V-N(1)	90.59(7)	O(2W)-V-N(1)	89.10(7)
O(1W)-V-O(1)	88.26(6)	O(2W)-V-O(1)	91.35(6)
O(1W)-V-O(2)	91.24(7)	O(2W)-V-O(2)	89.68(7)
O(1W)-V-O(5)	90.81(6)	O(2W)-V-O(5)	87.87(6)
O(1W)-V-O(7)	88.06(6)	O(2W)-V-O(7)	93.08(6)
N(1)-V-O(1)	149.85(6)	O(1)-V-O(2)	61.21(6)
N(1)-V-O(2)	148.94(6)	O(1)-V-O(5)	76.39(6)
N(1)-V-O(5)	73.51(6)	O(1)-V-O(7)	136.90(6)

N(1)-V-O(7)	73.11(6)	O(2)-V-O(5)	137.45(6)
O(7)-V-O(5)	146.59(6)	O(2)-V-O(7)	75.96(6)

Table S2. Hydrogen bonds (Å) and angles (°) of the complexes **1-2**.

Complex **1**				
D–H···A	d(D–H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
O9–H9B···O1$^{\#1}$	0.960	1.790	2.721(4)	162.7
O9–H9B···O5$^{\#1}$	0.960	2.418	3.009(4)	119.5
O10–H10B···O3$^{\#1}$	0.960	1.860	2.787(4)	161.5
O10–H10B···O6$^{\#1}$	0.960	2.362	3.016(4)	124.9
O10–H10A···O2$^{\#1}$	0.960	1.983	2.802(4)	141.9
O9–H9A···O2W$^{\#1}$	0.960	1.806	2.724(4)	158.8
O8–H8A···O2W$^{\#1}$	0.820	2.562	3.240(5)	140.9
O1W–H1WA···O8$^{\#1}$	0.820	2.127	2.785(5)	133.9
O1W–H1CW···O4$^{\#2}$	0.850	2.169	2.780(5)	128.6
Complex **2**				
O1W–H1A···O4$^{\#1}$	0.816(9)	1.808(9)	2.6224(19)	175(2)
O2W–H2A···O6$^{\#2}$	0.811(9)	1.919(9)	2.7187(19)	169(2)
O3–H3A···O1	0.82	1.85	2.588(3)	148.3

For **1**: #1= 1-x, -y, 1-z; #2=1-x, 1-y, 1-z. For **2**: #1= 1-x, 1-y, 1-z; #2= x, 0.5-y, -0.5+z

Table S3. IR data (cm^{-1}) for complexes **1**-**2**.

Complex	**1**	**2**
$\nu_{(O-H)}$	3417	3413
$\nu_{(C=CH)}$	3274, 3083	2973
$\nu_{(=C-CH)}$	934,875	925, 878
$\nu_{(-C-H)}$	746, 679,	753, 684
$\nu_{(COO^{-})}$	1624	1672
pyridine ring	1433, 1395, 1290, 1182 1076	1472, 1347, 1224, 1125, 1060
$\nu_{(V-Owater)}$	600, 562	585
$\nu_{(V-Ocarboxyl)}$	506	490
$\nu_{(V-N)}$	477	457

Table S4.Characteristic UV-vis absorption bands (nm) of the complexes **1**-**2**.

complex	**1**	**2**
π-π*	274, 324	274, 320
LMCT	386	378
d-d*	710	825

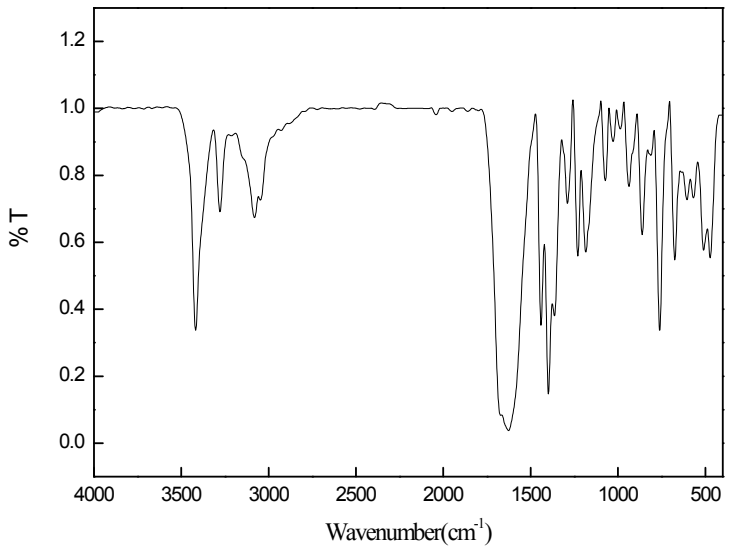

Fig S1. The Solid-state IR spectra of complex **1** at a room temperature

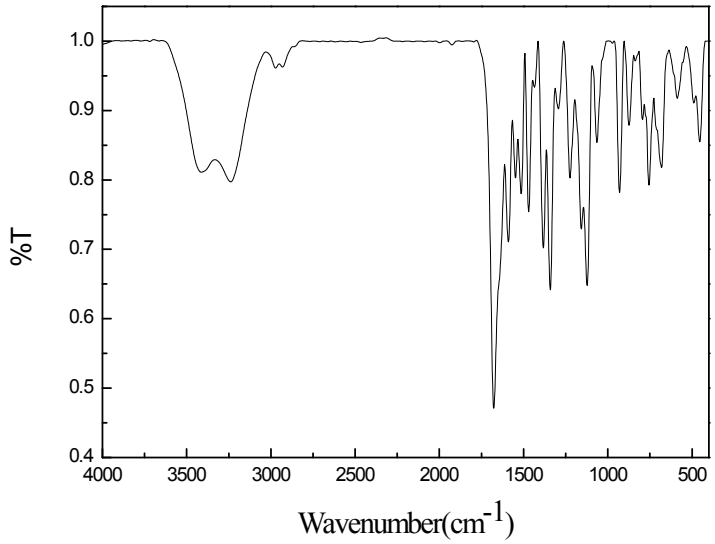

Fig S2. The Solid-state IR spectra of complex **2** at a room temperature

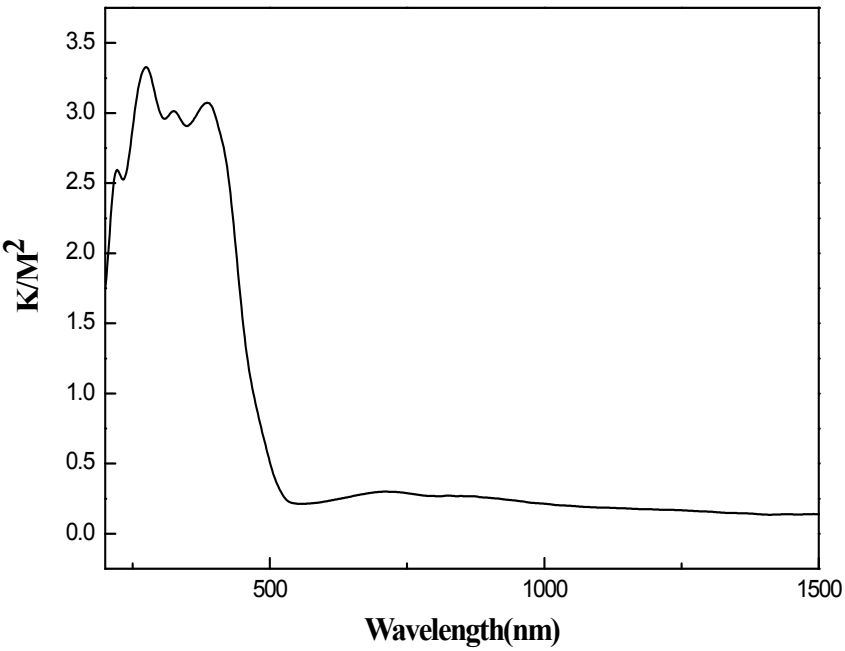

Fig S3. The Solid-state UV spectra of complex **1** at a room temperature

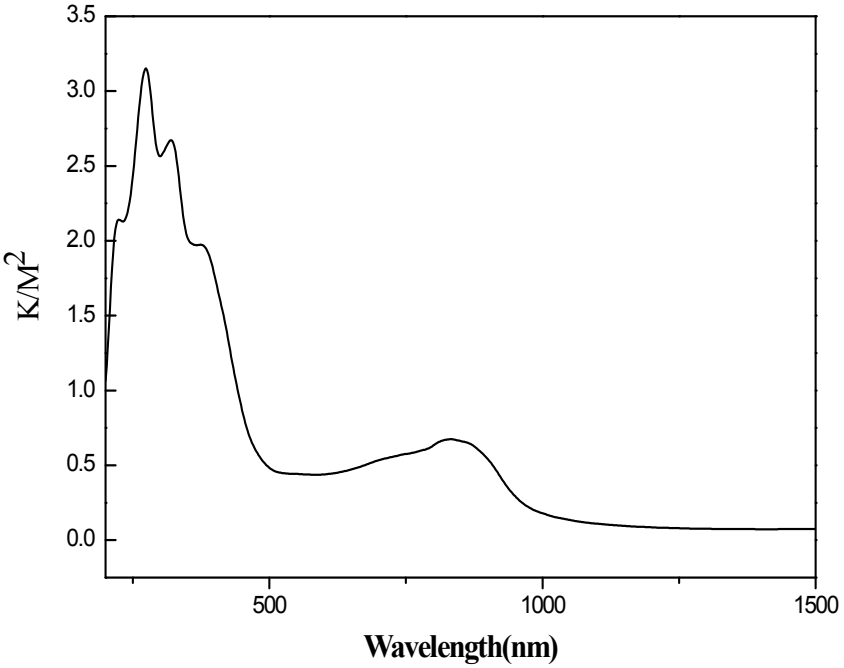

Fig S4. The Solid-state UV spectra of complex **2** at a room temperature

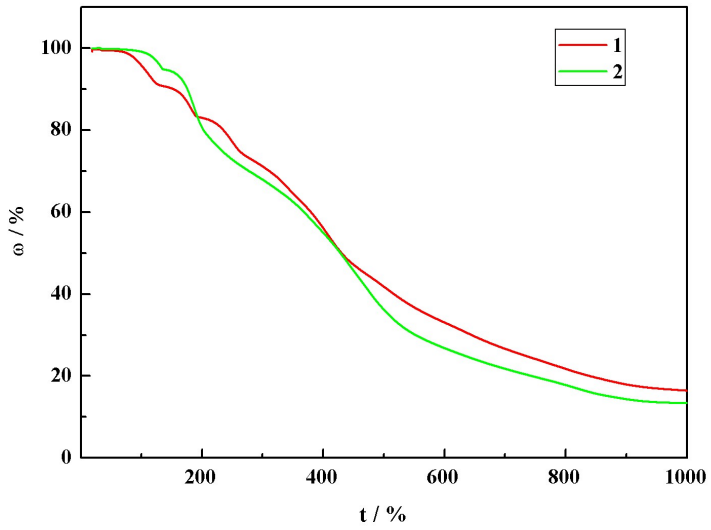

Fig S5. TG curves of the complexes **1**-**2**.

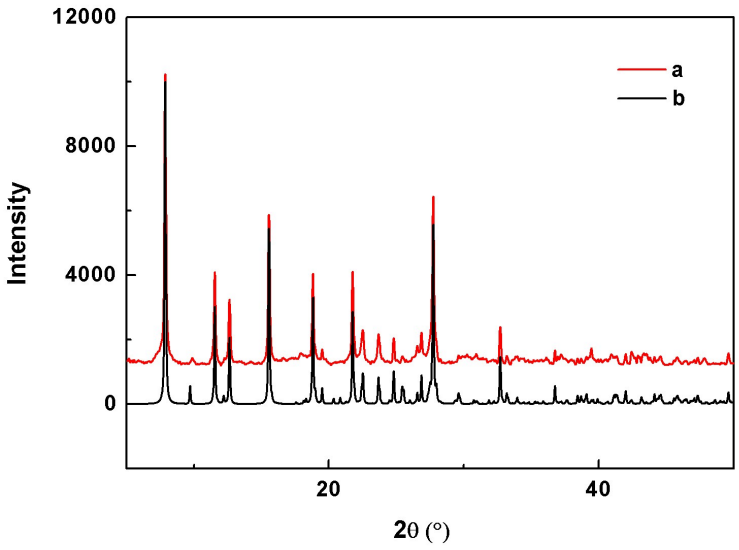

Fig.S6. The experimental XRD (a) and simulation XRD (b) spectrum of complex **1**.

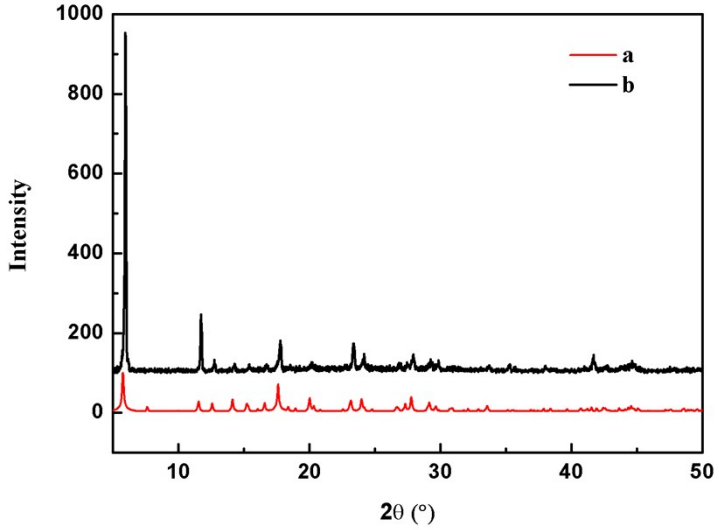

Fig.S7. The experimental XRD (a) and simulation XRD (b) spectrum of complex **2**.