

Supplementary Information

Synthesis, Structure and Characterization of Three Different Dimension Inorganic-Organic Hybrid Vanadates: [Co₂(mIM)₅(H₂O)₂]V₄O₁₂, [Ni₂(mIM)₇(H₂O)]V₄O₁₂·H₂O and [Cd(eIM)₂(H₂O)]V₂O₆

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Table S1. Crystallographic Data for Compound 1 -3

Compounds	Compound 1	Compound 2	Compound 3
Formula	C ₂₀ H ₃₄ Co ₂ N ₁₀ O ₁₄ V ₄	C ₂₈ H ₄₆ N ₁₄ Ni ₂ O ₁₄ V ₄	C ₁₀ H ₁₈ CdN ₄ O ₇ V ₂
M _r	960.19	1123.97	520.56
Crystal system	Orthorhombic	Triclinic	Monoclinic
Space group	P2 ₁ 2 ₁ 2 ₁	P-1	P2 ₁ /n
Temperature(K)	298(2)	298(2)	298(2)
a (Å)	11.4770(11)	9.4022(8)	9.4328(11)
b (Å)	17.8350(16)	13.4466(12)	16.3873(17)
c (Å)	17.8350(16)	17.5161(15)	11.3981(12)
α (deg)	90	89.367(2)	90
β (deg)	90	87.3580(10)	99.731
γ (deg)	90	87.4490(10)	90
V (Å ³)	3650.7(6)	2209.9(3)	1736.5(3)
Z	4	2	4
D _{calc.} (g cm ⁻³)	1.747	1.689	1.991
F(000)	1928	1144	1024
R ₁ [I>2σ(I)]	0.0843	0.0469	0.0329
wR ₂ [I>2σ(I)]	0.1929	0.0870	0.0603
R ₁ (all data)	0.1628	0.0825	0.0516
wR ₂ (all data)	0.2213	0.0954	0.0692
GOOF	1.054	1.021	1.065

Table S2. Selected bond distances (\AA) of Compound **1-3**

Compound 1		Compound 2		Compound 3	
Co(1)-N(2)	2.086(12)	Ni(1)-O(2)	2.043(3)	Cd(1)-N(4)	2.206(4)
Co(1)-N(4)	2.118(12)	Ni(1)-O(9)	2.046(3)	Cd(1)-N(2)	2.213(4)
Co(1)-O(11)	2.122(10)	Ni(1)-N(2)	2.060(4)	Cd(1)-O(6)	2.331(3)
Co(1)-O(13)	2.126(9)	Ni(1)-N(6)	2.067(4)	Cd(1)-O(2)	2.381(3)
Co(1)-N(6)	2.145(13)	Ni(1)-N(4)	2.073(4)	Cd(1)-O(2)#1	2.412(3)
Co(1)-O(3)	2.155(9)	Ni(1)-O(13)	2.107(3)	Cd(1)-O(7)	2.454(3)
Co(2)-O(14)	1.980(9)	Ni(2)-O(6)#1	2.056(3)	V(1)-O(3)	1.615(3)
Co(2)-N(10)	1.988(13)	Ni(2)-O(6)	2.056(3)	V(1)-O(2)	1.672(3)
Co(2)-N(8)	2.051(12)	Ni(2)-N(10)#1	2.086(4)	V(1)-O(1)	1.791(3)
Co(2)-O(2)	2.091(9)	Ni(2)-N(10)	2.086(4)	V(1)-O(4)	1.792(3)
Co(2)-O(8)	2.098(9)	Ni(2)-N(8)#1	2.105(4)	V(2)-O(5)	1.628(3)
V(1)-O(3)	1.649(9)	Ni(2)-N(8)	2.105(4)	V(2)-O(6)#1	1.644(3)
V(1)-O(2)	1.684(9)	Ni(3)-O(11)	2.068(3)	V(2)-O(4)#2	1.800(3)
V(1)-O(4)	1.803(9)	Ni(3)-O(11)#2	2.068(3)	V(2)-O(1)	1.805(3)
V(1)-O(1)	1.809(10)	Ni(3)-N(14)	2.085(4)		
V(2)-O(5)	1.594(10)	Ni(3)-N(14)#2	2.085(4)		
V(2)-O(6)	1.659(9)	Ni(3)-N(12)	2.120(4)		
V(2)-O(4)#1	1.814(9)	Ni(3)-N(12)#2	2.120(4)		
V(2)-O(1)	1.818(10)	V(1)-O(3)	1.623(4)		
V(3)-O(9)	1.625(10)	V(1)-O(2)	1.631(3)		
V(3)-O(8)	1.661(9)	V(1)-O(1)	1.760(3)		
V(3)-O(7)	1.784(9)	V(1)-O(4)#3	1.778(3)		
V(3)-O(10)	1.785(9)	V(2)-O(7)	1.618(4)		
V(4)-O(12)	1.633(9)	V(2)-O(6)	1.626(3)		
V(4)-O(11)	1.657(10)	V(2)-O(5)	1.776(4)		
V(4)-O(7)#2	1.831(9)	V(2)-O(1)	1.794(4)		
V(4)-O(10)#3	1.832(9)	V(3)-O(10)	1.612(3)		
O(4)-V(2)#4	1.814(9)	V(3)-O(9)	1.640(3)		
O(7)-V(4)#5	1.831(9)	V(3)-O(4)	1.784(3)		
O(10)-V(4)#6	1.832(9)	V(3)-O(8)	1.795(3)		
		V(4)-O(12)	1.618(4)		
		V(4)-O(11)	1.636(3)		
		V(4)-O(5)#4	1.775(3)		
		V(4)-O(8)	1.782(3)		

Symmetry transformations used to generate equivalent atoms: **(1)** #1 $x-1/2, -y+1/2, -z+1$; #2 $-x+3/2, -y, z+1/2$; #3 $-x+2, y+1/2, -z+3/2$; #4 $x+1/2, -y+1/2, -z+1$; #5 $-x+3/2, -y, z-1/2$; #6 $-x+2, y-1/2, -z+3/2$. **(2)** #1 $-x, -y+1, -z+1$; #2 $-x+2, -y+1, -z$; #3 $x-1, y, z$; #4 $x+1, y, z$. **(3)** #1 $-x+2, -y, -z+1$; #2 $-x+1, -y, -z+1$.

Table S3 Bond valance sum calculations

	Compound 1	Compound 2	Compound 3
V1 for compound 1	4.894	--	--
V2 for compound 1	5.144	--	--
V3 for compound 1	5.205	--	--
V4 for compound 1	4.916	--	--
Co1 for compound 1	2.339	--	--
Co2 for compound 1	2.359	--	--
V1 for compound 2	--	5.412	--
V2 for compound 2	--	5.363	--
V3 for compound 2	--	5.304	--
V4 for compound 2	--	5.356	--
Ni1 for compound 2	--	2.265	--
Ni2 for compound 2	--	2.248	--
Ni3 for compound 2		2.250	
V1 for compound 3	--	--	5.150
V2 for compound 3	--	--	5.144
Cd1 for compound 3	--	--	2.089

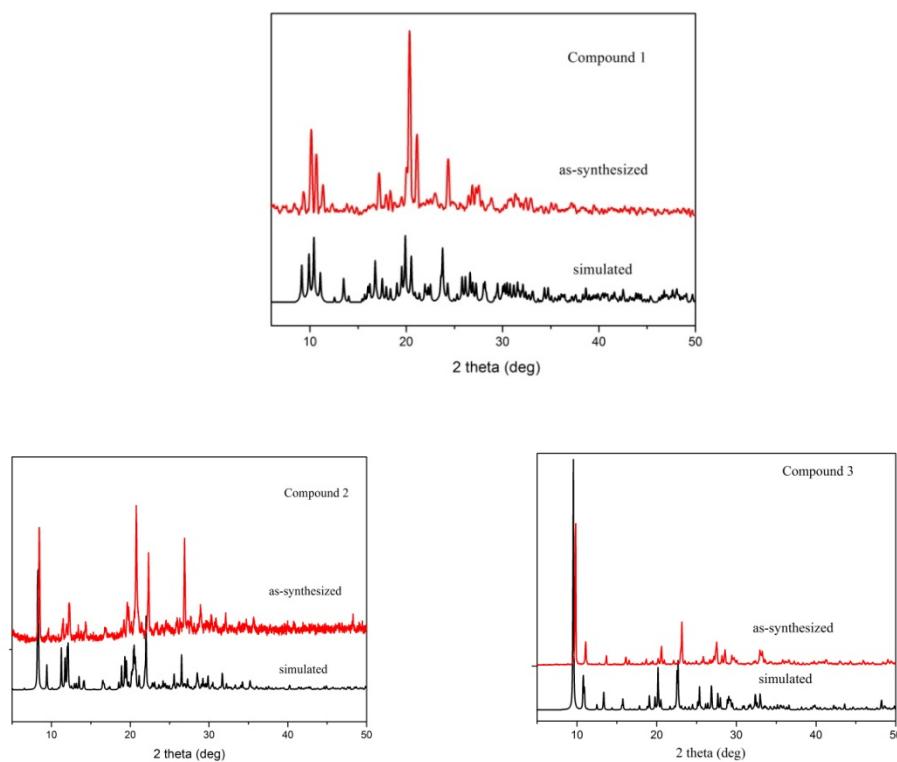


Fig. S1 The simulated (black) and experimental (red) powder XRD pattern of compound 1-3.

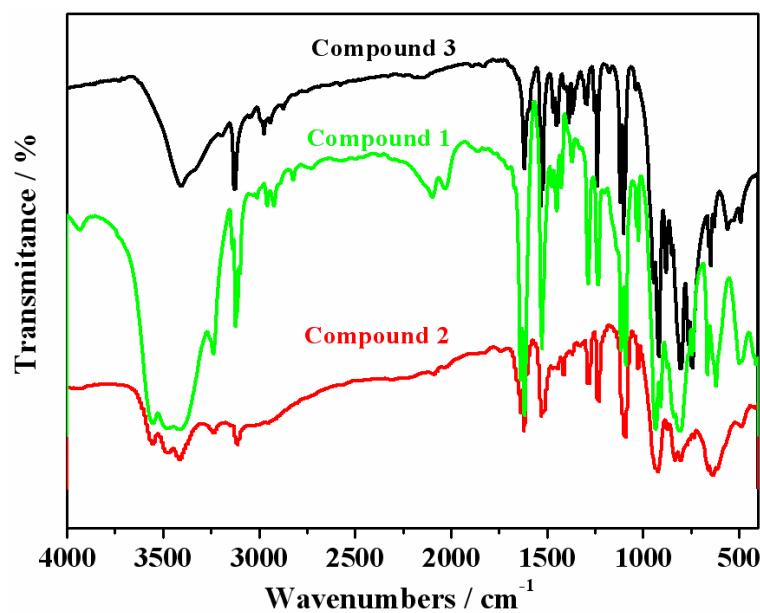


Fig. S2 The IR spectra of 1-3

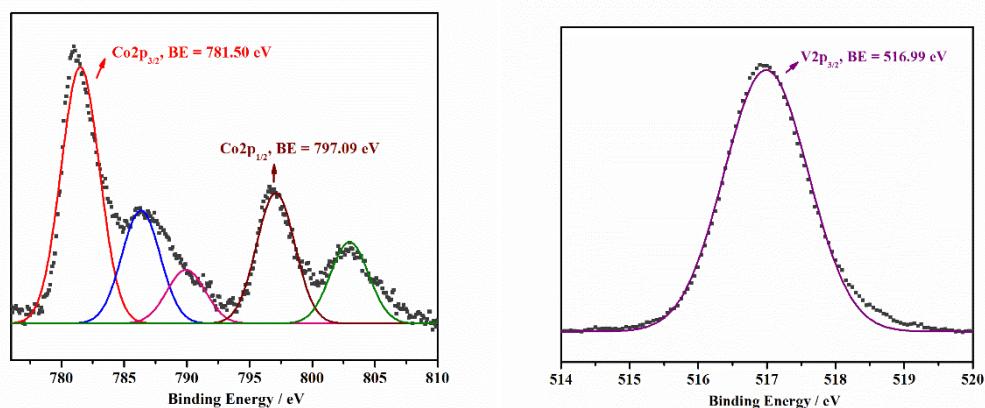


Fig.S3 XPS The XPS spectra for Co and V in 1

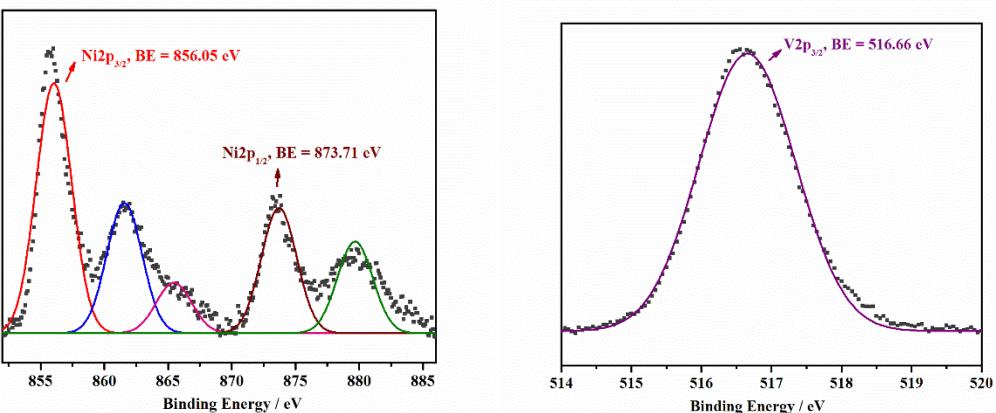


Fig.S4 XPS The XPS spectra for Ni and V in 2

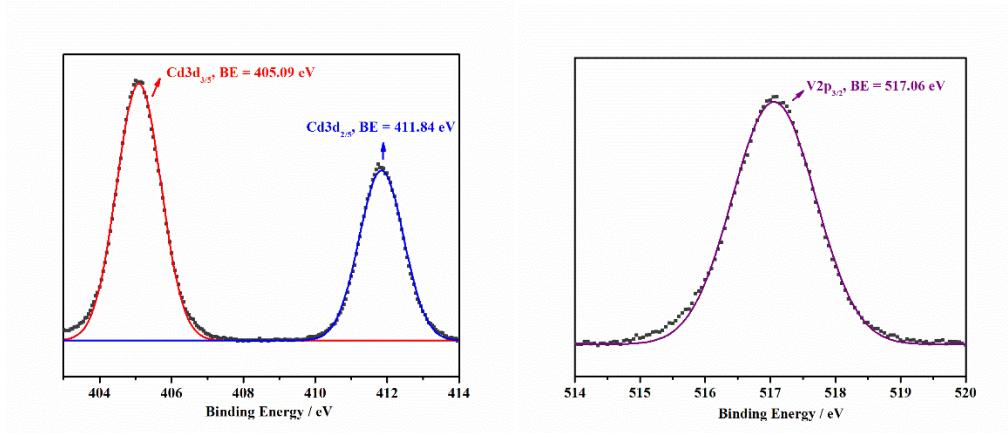


Fig.S5 The XPS spectra for Cd and V in 3

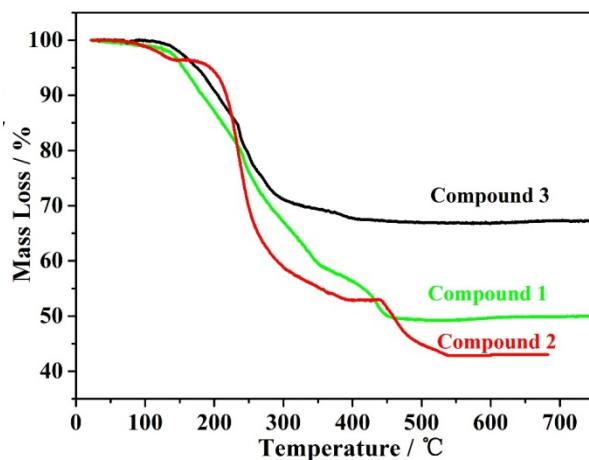


Fig. S6 Thermogavimetric Analysis of compound 1-3

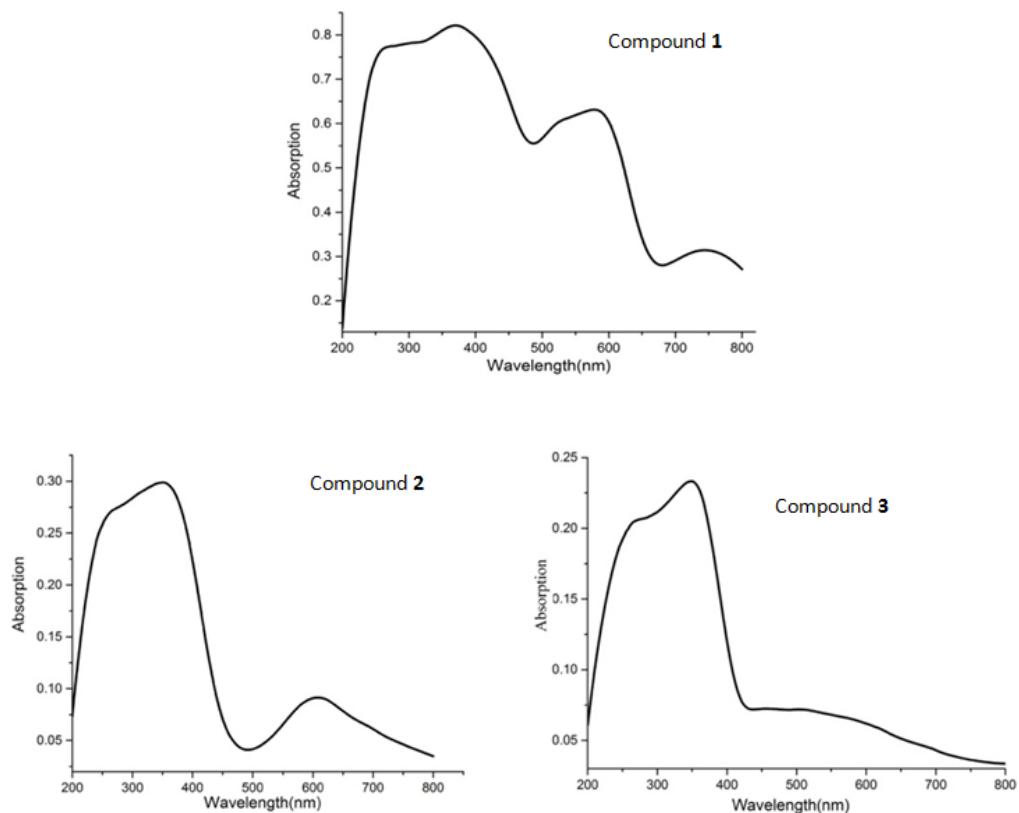


Fig. S7 The UV-vis absorption spectra of Compound 1-3