Supporting Information for

A 3-D chiral organic-inorganic hybrid zinc vanadate assembled from

helical units

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General Remarks

All analytical grade chemicals were obtained commercially and used without further purification. Elemental analyses (C, H, and N) were performed using a PE2400 II elemental analyzer. The UV/Vis spectra were recorded at room temperature using a computer-controlled PE Lambda 900 UV/Vis spectrometer equipped with an integrating sphere in the wavelength range of 250-800 nm. FT-IR spectra were recorded with a Nicolet Magna-IR 550 spectrometer in dry KBr disks in the 4000-400 cm⁻¹ range. The circular dichroism spectra were recorded on a JASCO J-810 Spectropolarimeter with KBr pellets. Powder XRD patterns were collected on a D/MAX-3C diffractometer using graphite-mono-chromatized CuKa radiation ($\lambda = 1.5406$ Å).

Synthesis of $[Zn_2(\mu-en)V_2O_7]_n$ (1)

A mixture of Na₂MoO₄ (0.1815g g), NH₄VO₃ (0.1185 g), Zn(CH₃COO)₂ (0.2592 g), ethylenediamine (en, 0.50mL) and water (1.7 mL) was stirred for 0.2 h, then final mixture with a pH of 10 was sealed in a 25 mL Teflon-lined autoclave and heated at 110 °C for 5 days. After cooling to room temperature slowly, pink-block crystals were isolated. The crystals were filtered and dried at room temperature (65 % yield based on NH₄VO₃). Anal. Calc for C₂H₈N₂O₇V₂Zn₂ for **1**: C, 5.94; H, 1.99; N, 6.92. Found. C,5.92; H, 2.01; N, 6.91. IR (cm⁻¹): 3258(m), 3190(m), 2947(w), 2899(w), 1596(s), 1570(s), 1317(m), 1216(m), 1169(m), 1121(m), 1021(s), 900(vs), 842(vs), 752(s), 657(m), 509(w), 472(w).

Crystal Structure Determination

Single-crystal X-ray diffraction data for **1** were recorded on a Rigaku Mercury CCD diffractometer using a ω -scan method with graphite monochromated Mo K α radiation ($\lambda = 0.71073$ Å) at 296(2) K to a maximum 2 θ value (50.18°). Absorption corrections were applied

using multi-scan technique. The structure of **1** was solved by Direct Method of SHELXS-97 and refined by full-matrix least-squares techniques using the SHELXL-97 program. Non-hydrogen atoms were refined with anisotropic temperature parameters. The H atoms bonded to C and N atoms were positioned with idealized geometry and refined with fixed isotropic displacement parameters. Relevant crystal and collection data parameters and refinement results can be found in Table S1. Additional details of crystal data in CIF format can be found in the Supporting Information. Selected Bond Lengths (Å) and Angles (deg) for **1** are listed in Table S2.

	1
formula	$C_2H_8N_2O_7V_2Zn_2$
Fw	404.76
crystal system	monoclinic
space group	$P2_{1}$
<i>a</i> , Å	7.0932(14)
<i>b</i> , Å	8.6150(17)
<i>c</i> , Å	8.1921(16)
β , deg	112.18(3)
<i>V</i> , Å ³	463.56(19)
Ζ	2
<i>Т</i> , К	296(2)
Calcd density,Mg.m ⁻³	2.900
abs coeff, mm ⁻¹	7.082
<i>F</i> (000)	392
$2\theta(\max), \deg$	50.18
Total reflns collected	2618
Unique reflns	1589
R _{int}	0.0175
No. of param	136

Table S1 Crystallographic data for 1.

$R1[I>2\sigma(I)]$	0.0173
wR2(all data)	0.0401
Flack parameter	0.030(13)
Goodness-of-fit	1.045

Table S2. Selected Bond Lengths (\AA) and Angles (deg) for 1.

Zn1-O3	1.961(3)	V1-O5	1.646(3)
Zn1-O1	1.966(2)	V1-O3	1.668(2)
Zn1-O2	1.980(2)	V1-O1#3	1.767(3)
Zn1-N1	2.015(3)	V1-O4	1.773(2)
Zn2-O6	1.958(2)	V2-O7#4	1.651(2)
Zn2-O1#1	2.005(2)	V2-O6	1.688(2)
Zn2-N2#2	2.024(3)	V2-O2#5	1.700(2)
Zn2-O5	2.144(3)	V2-O4#2	1.817(3)
Zn2-O7	2.196(2)		
O3-Zn1-O1	118.94(11)	O5-V1-O3	108.23(13)
O3-Zn1-O2	97.64(10)	O5-V1-O1#3	109.35(12)
O1-Zn1-O2	103.19(10)	O3-V1-O1#3	110.57(13)
O3-Zn1-N1	112.58(12)	O5-V1-O4	109.39(13)
O1-Zn1-N1	114.57(12)	O3-V1-O4	109.46(13)
O2-Zn1-N1	107.12(12)	O1#3-V1-O4	109.81(12)
O6-Zn2-O1#1	113.43(10)	O7#4-V2-O6	112.18(13)
O6-Zn2-N2#2	128.15(11)	O7#4-V2-O2#5	108.44(12)
O1#1-Zn2-N2#2	118.21(11)	O6-V2-O2#5	110.29(12)
O6-Zn2-O5	90.65(10)	O7#4-V2-O4#2	108.03(13)
O1#1-Zn2-O5	92.69(10)	O6-V2-O4#2	109.70(12)
N2#2-Zn2-O5	91.37(10)	O2#5-V2-O4#2	108.08(12)
O6-Zn2-O7	87.38(10)	N2#2-Zn2-O7	93.69(11)
O1#1-Zn2-O7	83.63(10)	O5-Zn2-O7	174.74(9)

Symmetry transformations used to generate equivalent atoms: (#1) x, y+1, z; (#2) -x+2,

y+1/2, -z+2; (#3) -x+1, y+1/2, -z+1; (#4) -x+2, y-1/2, -z+2; (#5) -x+1, y+1/2, -z+2.



Fig. S1 Simulated and experimental powder XRD patterns of 1.

The experimental peak positions are in agreement with simulated XRD pattern, indicating the phase purity of **1**. The difference in reflection intensity between experimental and simulated XRD patterns is probably due to the preferred orientation effect of the powder sample during collection of the experimental XRD data.



Fig. S2 3-D connection of the polyhedrons, showing bridging en molecules retained within the eight-membered channels (pink polyhedrons: $[ZnO_3N]/[ZnO_4N;$ blue polyhedrons: $[VO_4]$).



Fig. S3. The solid state UV–vis absorption spectrum of 1.



Fig. S4. The total density-of-states and partial density-of-states for **1**. The Fermi level is set at 0 eV (dotted line).



Fig. S5 Band structure for 1.