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Supporting information for article:

A potential Cu/V-organophosphonate platform for tailored void spaces *via* terpyridine mold casting

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Table of Contents

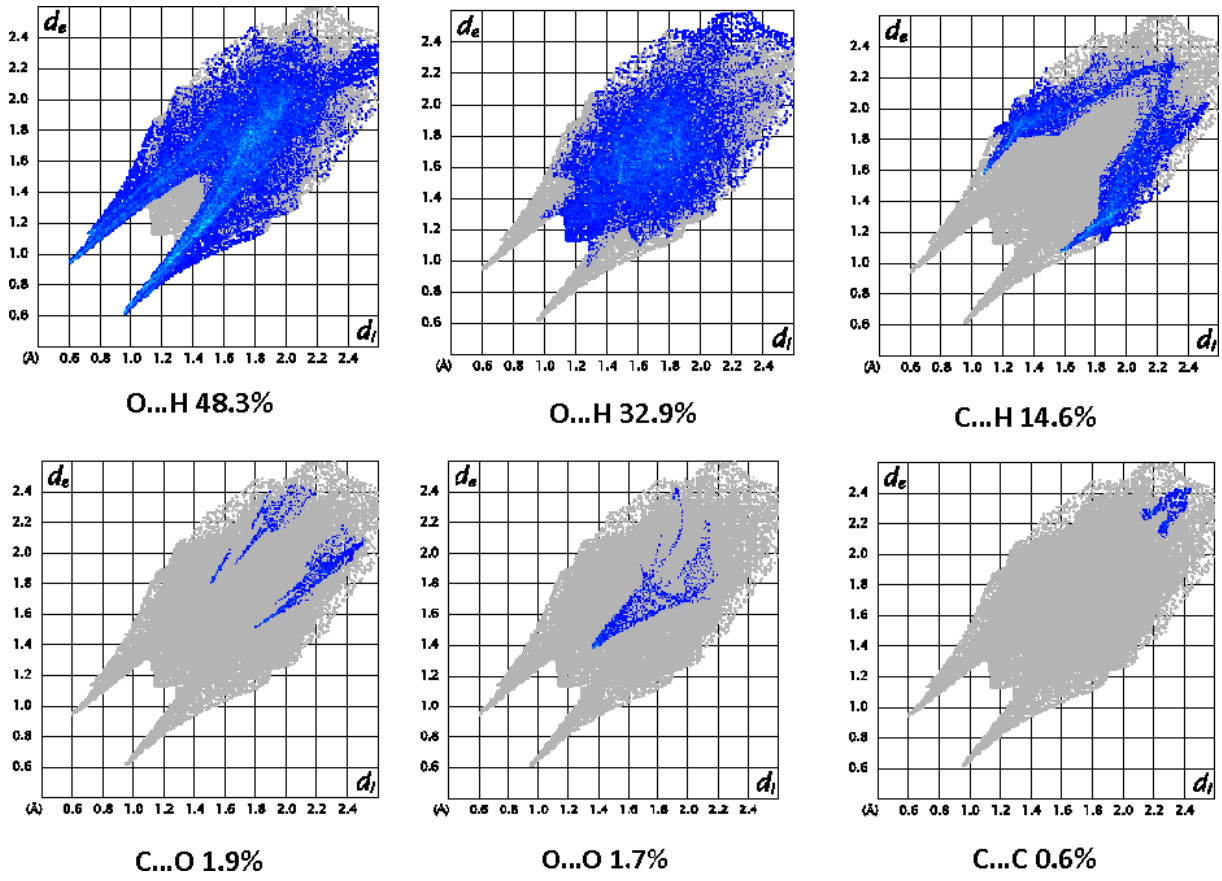

Figure S1 The resolved fingerprint plots of **MTPPA·MeOH** showing the percentage contribution of the O…H, H…H, C…H, C…O, O…O, C…C interactions to the total Hirshfeld surface area.

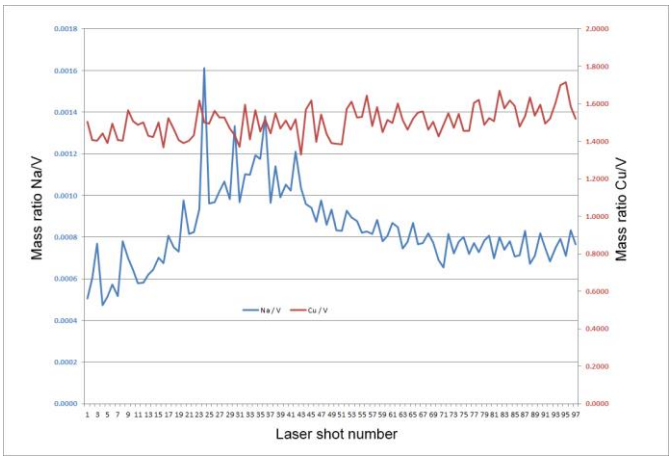

Figure S2 The depth profile of the Na/V and Cu/V mass percent ratio on a single crystal of **1** determined by Laser Ablation Inductive Coupled Plasma-Mass Spectroscopy (LA-ICP-MS)

showing that sodium is present only in trace amounts and the Cu/V-ratio is fairly constant throughout the crystal.

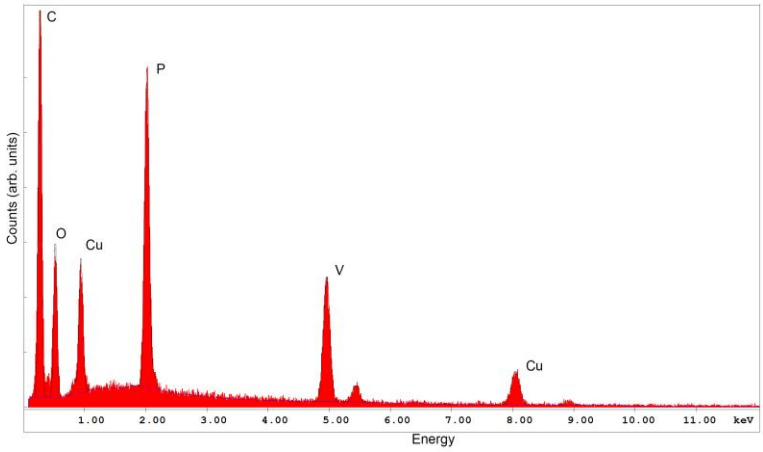

Figure S3 EDX analysis on a single crystal of **1**. No elements other than C, O, P, V and Cu can be detected.

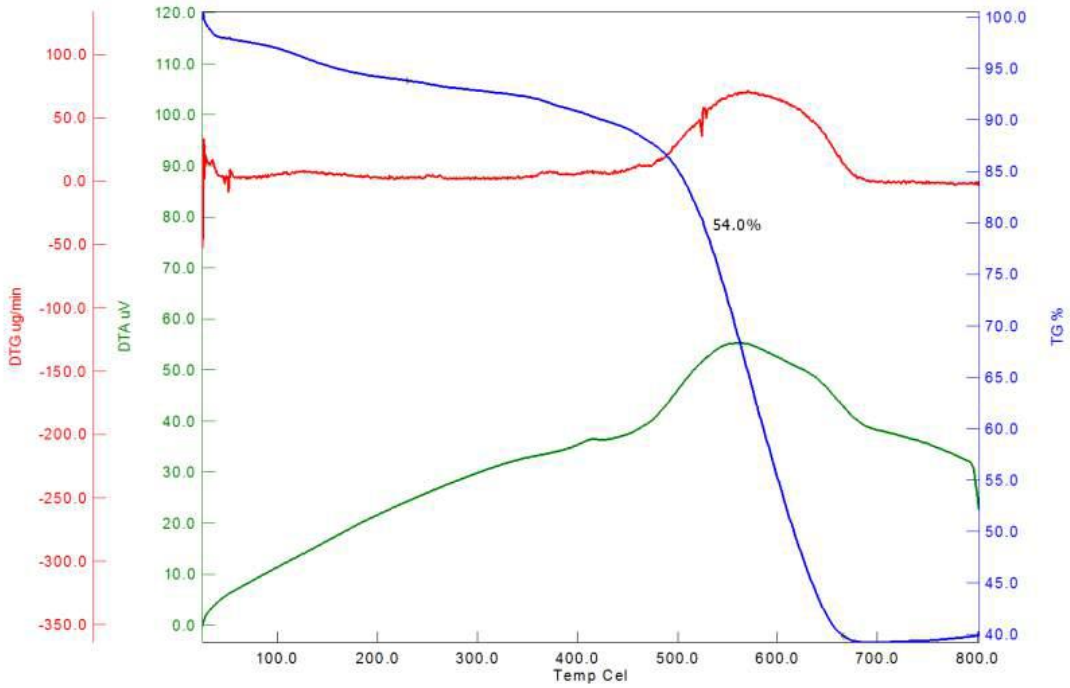

Figure S4 TGA curve of [{Cu(terpy)}$_4$Cu(VO$_2$)$_4$(MTPPA-H)$_2$]·4H$_2$O.

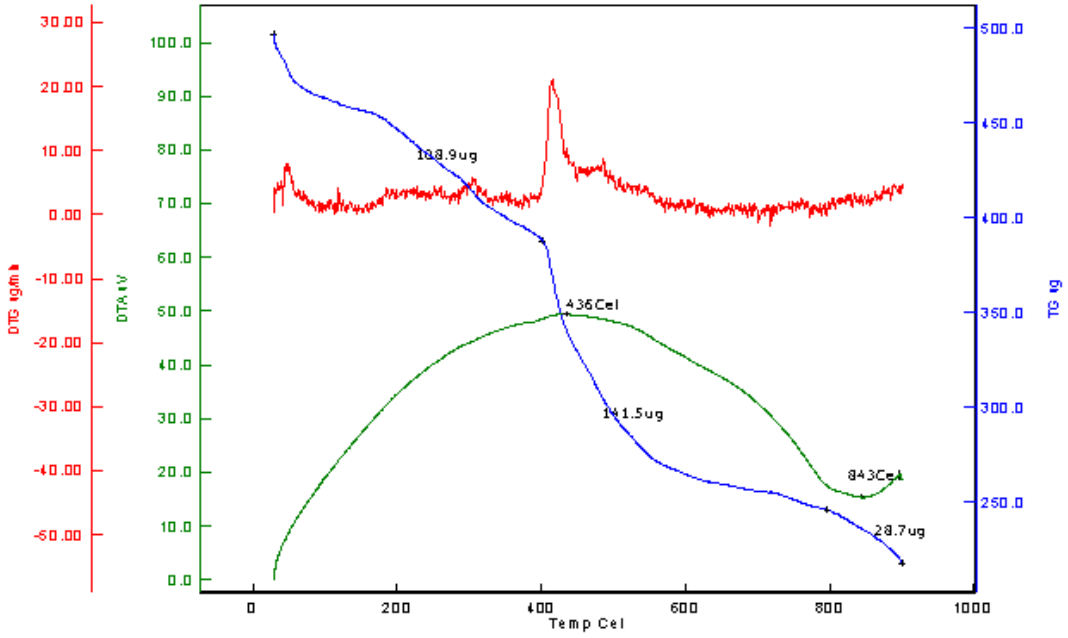

Figure S5 TGA curve of MTPPA·MeOH.

Table S1 Crystal data and structure refinement for **1** and MTPPA·MeOH.

Formula of refinement model	$C_{55}H_{42.47}Cu_{2.23}N_6O_{17.88}P_4V_{1.95}$	$C_{27}H_{32}O_{14}P_4$
Formula weight (g. mol^{-1})	1438.47	704.40
Temperature (K)	100(2)	296(2)
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*C*2/*c*
a/Å	13.6173(8)	29.093(3)
b/Å	14.3205(9)	7.2893(8)
c/Å	15.4896(9)	18.672(2)
α/°	77.4902(10)	90
β/°	71.7418(10)	127.610(5)
γ/°	76.5041(11)	90
Volume/Å^3	2755.4(3)	3136.8 (6)
Z	2	4
ρ_{calc}g/cm^3	1.734	1.492
μ/mm^{-1}	1.369	0.309
F(000)	1454.0	1464
Crystal size (mm)	0.33×0.16×0.06	0.11 × 0.10 × 0.06
Radiation and wavelength (Å)	MoKα (0.71073)	MoKα (0.71073)
θ range for data collection (°)	3.2 to 31.505	2.18 to 25.05
Index ranges	$-19 \le h \le 17$, $-20 \le k \le 20$, $-22 \le l \le 17$	$-34 \le h \le 34$, $-8 \le k \le 8$, $-22 \le l \le 22$

Reflections collected	22427	14601
Independent reflections	15399 [R_{int} = 0.0175]	2772 [R_{int} = 0.0526]
Data/restraints/parameters	15399/181/922	2772/102/262
Goodness-of-fit on F^2	1.07	1.08
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0467, wR_2 = 0.1147	R_1 = 0.0535, wR_2 = 0.1317
Final *R* indexes [all data]	R_1 = 0.0543, wR_2 = 0.1194	R_1 = 0.0703, wR_2 = 0.1410
Largest diff. peak and hole (e.Å^{-3})	1.33/-0.80	0.490/ -0.474