Electronic Supplementary Information (ESI)

New Journal of Chemistry

Influence of noncovalent interactions on the structures of metal–organic hybrids based on $[VO_2(2,6\text{-pydc})]^-$ tecton with cations of imidazole, pyridine and its derivatives

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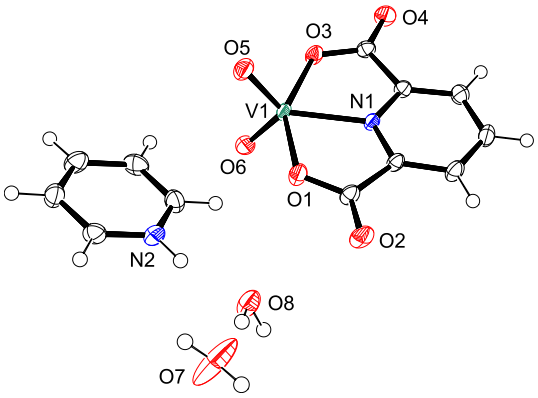

Fig. S1 Asymmetric unit of **1**·2H_2O.

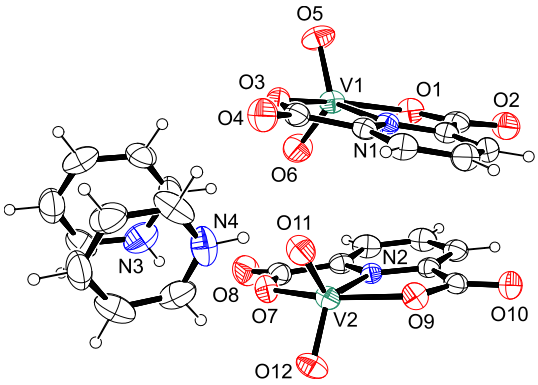

Fig. S2 Asymmetric unit of anhydrous **1**.

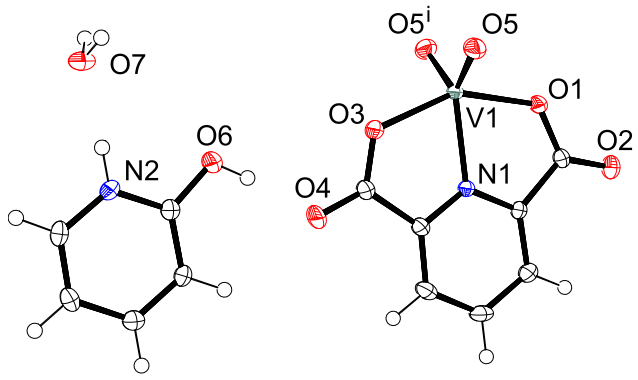

Fig. S3 Structure of **2**·H_2O. Symmetry code: (i) $x, -y + ½, z$.

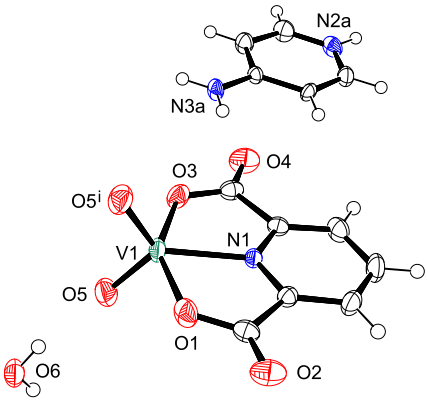

Fig. S4 Structure of **3**·H_2O. Symmetry code: (i) x, $-y + 1½$, z.

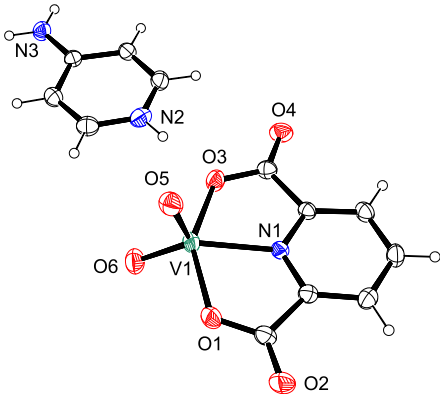

Fig. S5 Asymmetric unit of anhydrous **3**.

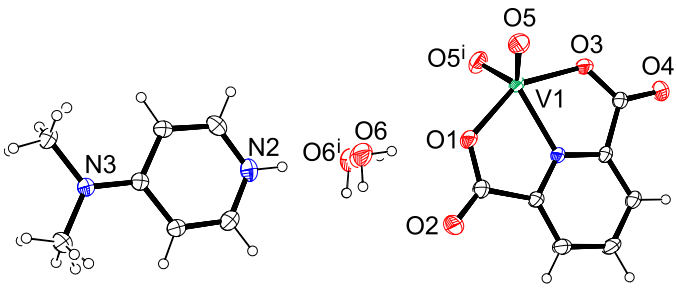

Fig. S6 Asymmetric unit of **4**·H_2O.

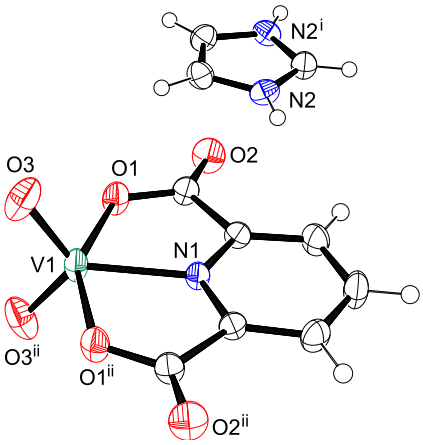

Fig. S7 Structure of **5**. Symmetry codes: (i) –*x* + 2, *y*, −*z* + 1; (ii) –*x* + 1, *y*, −*z* + 2.

Table S1. Selected bond distances for compounds **1–5**.

Distance	**1**·2H_2O [Å]	**1** [Å]	**2**·H_2O [Å]	**3**·H_2O [Å]	**3** [Å]	**4**·H_2O [Å]	**5** [Å]
V1–O1	1.9926(14)	1.992(3)	1.9783(17)	1.9865(19)	1.9914(14)	2.0013(17)	1.9803(12)
V1–O3	1.9985(14)	1.999(3)	2.0109(17)	1.9746(17)	2.0051(13)	1.9869(16)	1.6212(15)
V1–O5	1.6299(14)	1.603(3)	1.6212(13)	1.6186(13)	1.6078(14)	1.6133(13)	
V1–O6	1.6127(15)	1.612(3)			1.6311(14)		
V1–N1	2.0941(15)	2.087(3)	2.0848(19)	2.0941(18)	2.0993(13)	2.0912(18)	2.0824(19)
V2–O7		1.989(3)					
V2–O9		1.981(3)					
V2–O11		1.603(3)					
V2–O12		1.619(3)					
V2–N2		2.088(3)					
O1–C1	1.296(2)	1.282(5)	1.305(3)	1.302(3)	1.291(2)	1.294(3)	1.298(2)
O2–C1	1.224(2)	1.226(5)	1.217(3)	1.213(3)	1.222(2)	1.213(3)	1.213(2)
O3–C7	1.292(2)	1.303(5)	1.281(3)	1.299(3)	1.309(2)	1.304(3)	
O4–C7	1.224(2)	1.222(5)	1.234(3)	1.215(3)	1.212(2)	1.211(3)	
O7–C8		1.310(5)					
O8–C8		1.210(5)					
O9–C14		1.294(5)					
O10–C14		1.217(5)					

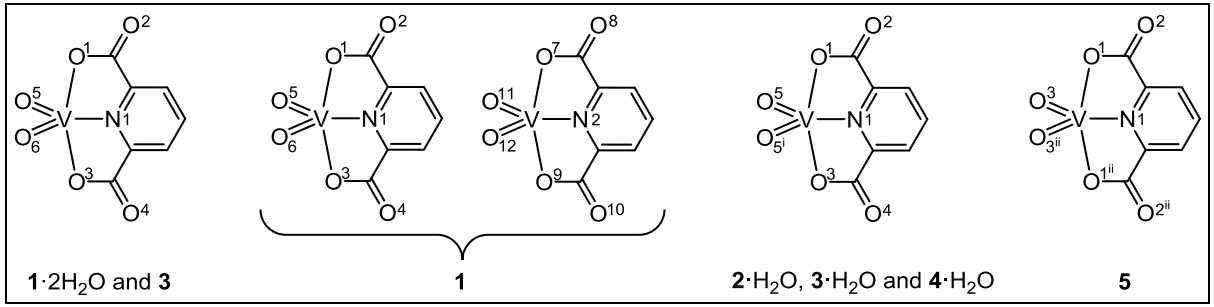

Table S2. Selected bond angles for compounds **1**–**5**.

Angle		**1**·2H$_2$O [°]	**1** [°]	**3** [°]
O1–V1–O3		148.95(6)	148.71(12)	147.97(5)
O1–V1–O5		98.85(7)	100.15(15)	98.95(7)
O1–V1–O6		99.27(7)	98.98(15)	100.64(7)
O3–V1–O5		98.55(7)	98.13(16)	99.66(7)
O3–V1–O6		98.93(7)	97.92(15)	98.11(7)
O5–V1–O6		109.37(8)	110.85(18)	107.92(7)
N1–V1–O1		74.59(6)	74.38(12)	74.86(5)
N1–V1–O3		74.43(6)	74.36(12)	73.86(5)
N1–V1–O5		128.17(7)	123.73(15)	113.63(7)
N1–V1–O6		122.46(7)	125.40(14)	138.42(7)
O7–V2–O9			148.89(12)	
O7–V2–O11			97.25(14)	
O7–V2–O12			98.90(15)	
O9–V2–O11			99.29(15)	
O9–V2–O12			99.78(14)	
O11–V2–O12			110.30(17)	
N2–V2–O7			74.45(12)	
N2–V2–O9			74.49(11)	
N2–V2–O11			125.37(14)	
N2–V2–O12			124.31(14)	

Angle		**2**·H$_2$O [°]	**3**·H$_2$O [°]	**4**·H$_2$O [°]
O1–V1–O3		149.16(7)	148.86(7)	149.22(7)
O1–V1–O5		99.01(5)	98.55(6)	98.39(5)
O3–V1–O5		98.66(5)	99.59(6)	99.20(5)
O5–V1–O5^{i}		109.39(9)	108.07(10)	109.66(10)
N1–V1–O1		74.71(7)	73.94(7)	74.53(7)
N1–V1–O3		74.45(7)	74.93(7)	74.69(7)
N1–V1–O5		125.30(5)	125.95(5)	125.17(5)
Symmetry code:		(i) x, $-y + ½$, z	(i) x, $-y + 1½$, z	(i) x, y, $-z + ½$

Angle		**5** [°]
O1–V1–O1^{ii}		150.04(7)
O1–V1–O3		98.52(7)
O1–V1–O3^{ii}		98.43(6)
O3–V1–O3^{ii}		110.49(13)
N1–V1–O1		75.02(4)
N1–V1–O3		124.76(6)
Symmetry code:		(ii) $–x + 1$, y, $–z + 2$

Table S3 Hydrogen bonds for **1**·2H_2O and anhydrous **1** [Å and °]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry transformation for acceptors
1·2H_2O					
N2–H2···O8	0.88	1.80	2.661(2)	167	*x*, *y*, *z*
O7–H7A···O4	0.83(2)	1.99(2)	2.807(2)	169(5)	*x*, *y* + 1, *z* + 1
O7–H7B···O5	0.83(2)	2.03(3)	2.796(2)	153(5)	−*x*, −*y* + 1, −*z* + 1
O8–H8A···O2	0.84(2)	2.09(2)	2.877(2)	158(3)	−*x* + 1, −*y* + 2, −*z* + 1
O8–H8B···O7	0.84(2)	1.83(2)	2.670(3)	173(3)	*x*, *y*, *z*
C3–H3···O6	0.95	2.41	3.208(2)	142	*x*, *y* + 1, *z*
C5–H5···O5	0.95	2.57	3.202(2)	124	–*x*, –*y* + 1, –*z*
C5–H5···O6	0.95	2.58	3.271(2)	130	–*x* + 1, –*y* + 1, –*z*
C8–H8···O1	0.95	2.25	3.150(3)	157	*x*, *y*, *z*
C10–H10···O2	0.95	2.56	3.231(3)	128	*x* + 1, *y* – 1, *z*
1					
N3–H3*N*···O7	0.86	2.54	3.129 (6)	126	*x*, *y*, *z*
N4–H4*N*···O11	0.86	2.19	2.876 (6)	137	*x*, *y*, *z*
C10–H10···O12	0.93	2.49	3.402(5)	166	*x* – 1, *y*, *z*
C15–H15···O3	0.93	2.58	3.218(6)	126	*x*, *y*, *z*
C21–H21···O5	0.93	2.58	3.476(6)	163	–*x* + 1, –*y* + 1, –*z* + 1
C22–H22···O10	0.93	2.53	3.403(7)	156	*x* + 1, *y* – 1, *z*
C23–H23···O7	0.93	2.56	3.412(6)	153	–*x* + 1, –*y* + 1, –*z*

Table S4 Hydrogen bonds for **2**·H_2O [Å and °]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry transformation for acceptors
N2–H2···O7	0.88	1.80	2.677(3)	177	*x*, *y*, *z*
O6–H6*O*···O4	0.84	1.74	2.577(2)	175	*x*, *y*, *z*
O7–H7*O*···O5	0.83(1)	2.00(1)	2.8090(18)	166(2)	−*x* + 1, −*y* + 1, −*z* + 1
C3–H3···O5	0.95	2.56	3.280(2)	132	–*x* + 1, –*y* + 1, –*z*
C3–H3···O5	0.95	2.56	3.280(2)	132	–*x* + 1, *y* – ½, –*z*
C5–H5···O1	0.95	2.40	3.144(3)	135	*x* + 1, *y*, *z*
C8–H8···O2	0.95	2.55	3.475(3)	164	*x* + 1, *y*, *z* + 1
C10–H10···O3	0.95	2.55	3.442(3)	157	*x* + 1, *y*, *z*
C11–H11···O4	0.95	2.50	3.143(3)	125	*x*, *y*, *z*

Table S5 Hydrogen bonds for **3**·H_2O and anhydrous **3** [Å and °]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry transformation for acceptors
3·H_2O					
O6–H6*O*···O5	0.84	1.93	2.7624(18)	168	*x*, *y*, *z*
N2*A*–H2*A*···O1	0.88	1.89	2.765(4)	173	*x*, *y*, *z* − 1
N3*A*–H3*A*···O4	0.88	1.97	2.844(3)	176	*x*, *y*, *z*
N3*A*–H3*B*···O6	0.88	1.94	2.819(4)	175	−*x*, *y* + ½, −*z* + 1
N2*B*–H2*B*···O6	0.88	1.94	2.770(8)	156	−*x*, *y* + ½, −*z* + 1
N3*B*–H3*C*···O6	0.88	2.11	2.978(7)	169	−*x* + 1, *y* + ½, −*z* + 1
N3*B*–H3*D*···O1	0.88	2.28	3.130(7)	164	*x*, *y*, *z* − 1
N3*B*–H3*D*···O2	0.88	2.43	3.153(8)	140	*x*, *y*, *z* − 1
3					
N2–H2···O3	0.86	1.92	2.783(2)	178	*x*, *y*, *z*
N3–H3*A*···O6	0.86	2.15	3.004(2)	170	−*x* + 1, *y* + ½, −*z* + ½
N3–H3*B*···O2	0.86	2.04	2.888(2)	171	*x* − 1, −*y* + ½, *z* − ½
C3–H3···O6	0.93	2.57	3.477(3)	165	–*x* + 2, *y* – ½, –*z* + 1½
C8–H8···O5	0.93	2.48	3.084(3)	122	–*x* + 1, –*y*, –*z* + 1
C12–H12···O4	0.93	2.55	3.230(3)	130	*x*, –*y* + ½, *z* – ½

Table S6 Hydrogen bonds for **4**·H_2O [Å and °]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry transformation for acceptors
N2–H2···O6	0.86	1.98	2.824(3)	168	*x*, *y*, *z*
N2–H2···O6	0.86	1.98	2.824(3)	168	*x*, *y*, −*z* + 1½
O6–H6A···O5	0.82(1)	2.38(3)	3.071(3)	144(5)	*x*, −*y* + 1½, −*z* + 1
O6–H6B···O1	0.82(1)	2.33(2)	3.140(3)	169(5)	*x*, *y*, *z*
O6–H6B···O2	0.82(1)	2.53(4)	3.080(3)	126(4)	*x*, *y*, *z*
C8–H8···O2	0.93	2.38	3.222(3)	151	*x* + 1, *y*, *z*
C11–H11···O4	0.93	2.43	3.358(3)	173	–*x* + 1, *y* – ½, –*z* + 1½
C14–H14B···O3	0.96	2.56	3.463(3)	157	–*x* + 2, *y* – ½, –*z* + 1½

Table S7 Hydrogen bonds for **5** [Å and °]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry transformation for acceptors
N2–H2N···O2	0.86	2.24	2.8288 (19)	126	*x*, *y*, *z*
N2–H2N···O3	0.86	2.12	2.801 (2)	135	*x* + ½, *y* + ½, *z*
C3–H3···O3	0.93	2.46	3.359(4)	162	*x* + ½, *y* + ½, *z*
C5–H5···O1	0.93	2.58	3.323(3)	137	*x* + ½, *y* + ½, *z*
C5–H5···O1	0.93	2.58	3.323(3)	137	–*x* + 1½, *y* + ½, –*z* + 1

Table S8 Geometrical parameters (Å, °) for π···π stacking interactions in **1**·2H_2O, **1**, **4**·H_2O and **5**

*Cg*I···*Cg*J	*Cg*I···*Cg*J	*α*	*β* (*γ*)	*Cg*I-Perp (offset distance)	Ring slippage	Symmetry transformation for acceptors
1·2H_2O						
*Cg*4···*Cg*4	4.1093(13)	0	51.30	3.0515(8)	3.809	–*x*, –*y* + 1, –*z* + 1
*Cg*4 is N2/C8–C12 ring centroid.						
1						
*Cg*7···*Cg*8	3.878(4)	6.3(3)	18.28, 16.77	–3.713(2)	/	*x*, *y*, *z*
*Cg*7···*Cg*8	4.230(4)	6.3(3)	30.27, 34.12	3.502(2)	/	*x* – 1, *y*, *z*
*Cg*7 and *Cg*8 are N3/C15–C19 and N4/C20–C24 ring centroids, respectively.						
4·H_2O						
*Cg*3···*Cg*4	3.8718(7)	0	30.97	3.3199	1.992	*x* – 1, –*y* + 1½, –*z* + 1
*Cg*3 and *Cg*4 are N1/C2–C6 and N2/C8–C12 ring centroids, respectively.						
5						
*Cg*3···*Cg*4	3.6787(13)	0.34(10)	25.01, 25.31	3.3255(7)	/	*x*, *y*, *z* + 1
*Cg*3 and *Cg*4 are N1/C2–C4/C3[a]/C2[a] and N2/C5/N2[b]/C6[b]/C6 ring centroids, respectively. Symmetry codes: (a) –*x* + 1, *y*, −*z* + 2; (b) –*x* + 2, *y*, −*z* + 1.						

CgI···CgJ, *α, β, γ* and CgI-Perp are the centroid-to-centroid distance between rings I and J (Å), the inter-ring dihedral angle (°), slip angles (°), and the perpendicular distance of CgI from ring J (Å) , respectively. Ring slippage is in Å.

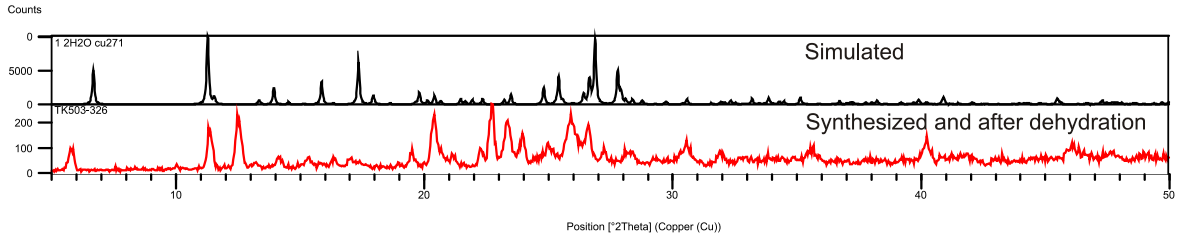

Fig. S8 Comparison of PXRD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product after dehydration of **1**·2H_2O to **1**·H_2O.

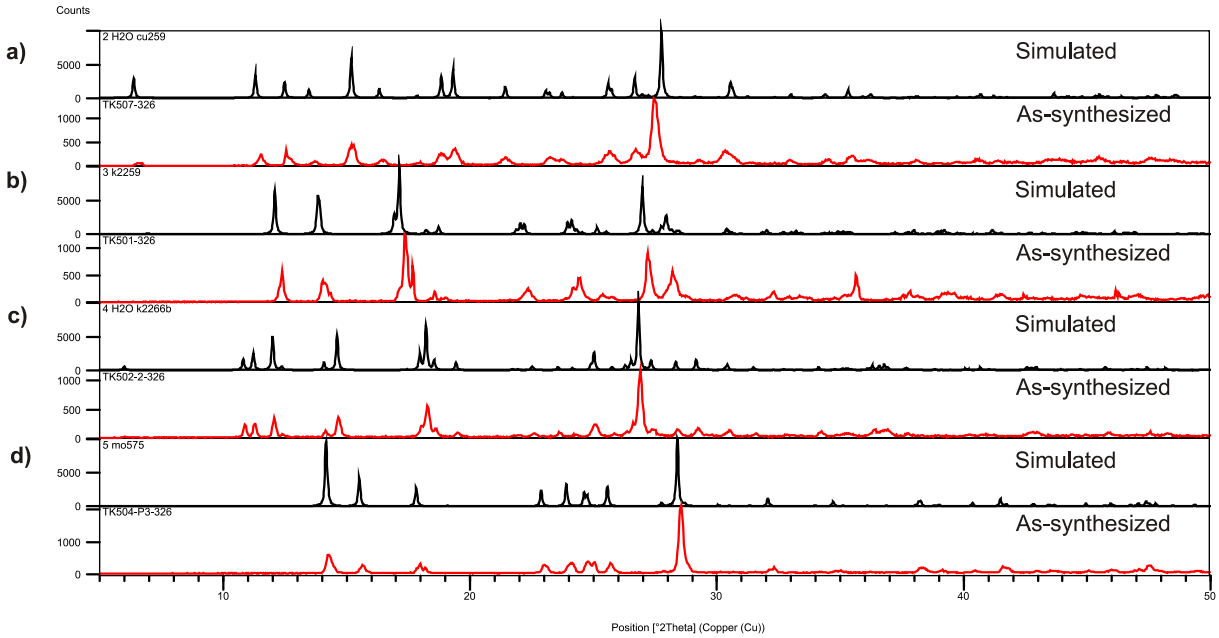

Fig. S9 Comparison of PXRD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized products in compounds a) **2**·H_2O, b) **3**, c) **4**·H_2O and d) **5**.