

Supplementary Material (ESI) for RSC Advances
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A novel polyoxometalate templated microporous metal–organic framework with electrochemical properties†

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Table S1. Selected bond distances (Å) and angles (°) for compound 1

Cu(1)-N(1)#1	2.043(6)	W(3)-O(8)	1.707(5)
Cu(1)-N(1)	2.043(6)	W(3)-O(7)#6	1.864(5)
Cu(1)-N(1)#2	2.043(6)	W(3)-O(6)	1.900(5)
Cu(1)-N(1)#3	2.043(6)	W(3)-O(5)	1.915(5)
Cu(1)-O(1W)	2.411(14)	W(3)-O(6)#5	1.962(5)
W(1)-O(10)	1.713(5)	W(3)-O(1)	2.389(4)
W(1)-O(3)	1.880(5)	P(1)-O(2)#6	1.527(5)
W(1)-O(5)	1.902(5)	P(1)-O(2)	1.527(5)
W(1)-O(11)	1.917(5)	P(1)-O(2)#5	1.527(5)
W(1)-O(4)	1.931(5)	P(1)-O(1)	1.560(8)
W(1)-O(2)	2.369(5)	O(1)-W(3)#5	2.389(4)
W(2)-O(9)	1.728(5)	O(1)-W(3)#6	2.389(4)
W(2)-O(4)#5	1.869(5)	O(4)-W(2)#6	1.869(5)
W(2)-O(11)#4	1.879(5)	O(6)-W(3)#6	1.962(5)
W(2)-O(3)	1.925(5)	O(7)-W(3)#5	1.864(5)
W(2)-O(7)	1.967(5)	O(11)-W(2)#4	1.879(5)
W(2)-O(2)	2.368(5)	N(1)#1-Cu(1)-N(1)	89.971(11)
N(1)#1-Cu(1)-N(1)#2	89.971(11)	O(9)-W(2)-O(7)	97.6(2)
N(1)-Cu(1)-N(1)#2	177.4(4)	O(4)#5-W(2)-O(7)	86.2(2)
N(1)#1-Cu(1)-N(1)#3	177.4(4)	O(11)#4-W(2)-O(7)	163.3(2)
N(1)-Cu(1)-N(1)#3	89.971(10)	O(3)-W(2)-O(7)	86.7(2)
N(1)#2-Cu(1)-N(1)#3	89.971(11)	O(9)-W(2)-O(2)	172.9(2)
N(1)#1-Cu(1)-O(1W)	91.3(2)	O(4)#5-W(2)-O(2)	84.93(19)
N(1)-Cu(1)-O(1W)	91.3(2)	O(11)#4-W(2)-O(2)	83.00(19)
N(1)#2-Cu(1)-O(1W)	91.3(2)	O(3)-W(2)-O(2)	72.50(19)
N(1)#3-Cu(1)-O(1W)	91.3(2)	O(7)-W(2)-O(2)	80.30(19)

O(10)-W(1)-O(3)	100.4(3)	O(8)-W(3)-O(7)#6	103.9(2)
O(10)-W(1)-O(5)	97.9(2)	O(8)-W(3)-O(6)	100.6(3)
O(3)-W(1)-O(5)	93.0(2)	O(7)#6-W(3)-O(6)	90.5(2)
O(10)-W(1)-O(11)	98.3(2)	O(8)-W(3)-O(5)	102.7(3)
O(3)-W(1)-O(11)	91.3(2)	O(7)#6-W(3)-O(5)	86.9(2)
O(5)-W(1)-O(11)	162.2(2)	O(6)-W(3)-O(5)	156.5(2)
O(10)-W(1)-O(4)	102.5(3)	O(8)-W(3)-O(6)#5	99.0(2)
O(3)-W(1)-O(4)	157.0(2)	O(7)#6-W(3)-O(6)#5	157.0(2)
O(5)-W(1)-O(4)	85.1(2)	O(6)-W(3)-O(6)#5	87.2(3)
O(11)-W(1)-O(4)	84.2(2)	O(5)-W(3)-O(6)#5	86.2(2)
O(10)-W(1)-O(2)	173.6(3)	O(8)-W(3)-O(1)	170.0(2)
O(3)-W(1)-O(2)	73.2(2)	O(7)#6-W(3)-O(1)	84.64(19)
O(5)-W(1)-O(2)	82.13(19)	O(6)-W(3)-O(1)	73.73(19)
O(11)-W(1)-O(2)	82.59(19)	O(5)-W(3)-O(1)	82.77(18)
O(4)-W(1)-O(2)	83.9(2)	O(6)#5-W(3)-O(1)	72.73(19)
O(9)-W(2)-O(4)#5	101.7(2)	O(2)#6-P(1)-O(2)	111.90(18)
O(9)-W(2)-O(11)#4	99.0(3)	O(2)#6-P(1)-O(2)#5	111.90(18)
O(4)#5-W(2)-O(11)#4	92.1(2)	O(2)-P(1)-O(2)#5	111.90(18)
O(9)-W(2)-O(3)	100.7(2)	O(2)#6-P(1)-O(1)	106.9(2)
O(4)#5-W(2)-O(3)	157.2(2)	O(2)-P(1)-O(1)	106.9(2)
O(11)#4-W(2)-O(3)	88.5(2)	O(2)#5-P(1)-O(1)	106.9(2)

Symmetry code: #1 $z, y, -x + 1$; #2 $-x + 1, y, -z + 1$; #3 $-z + 1, y, x$; #4 $-x + 1/2, -z + 3/2, -y + 3/2$; #5 $-z + 1, -x + 1, y$; #6 $-y + 1, z, -x + 1$.

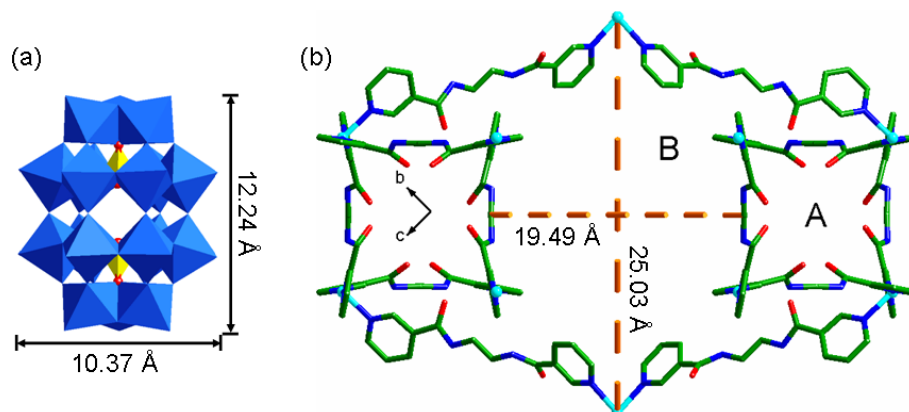


Fig. S1 (a) Polyhedral representation of the P_2W_{18} anion. (b) Representation of the channels A and B in the 3D net viewed along the a -axis.

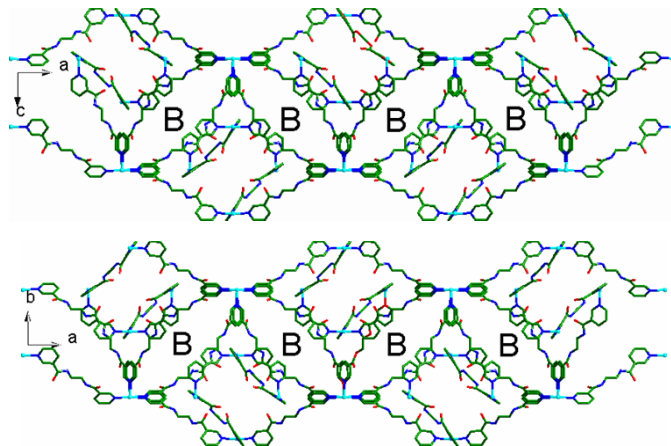


Fig. S2 Representations of the channels B in the 3D net viewed along the b/c -axis.

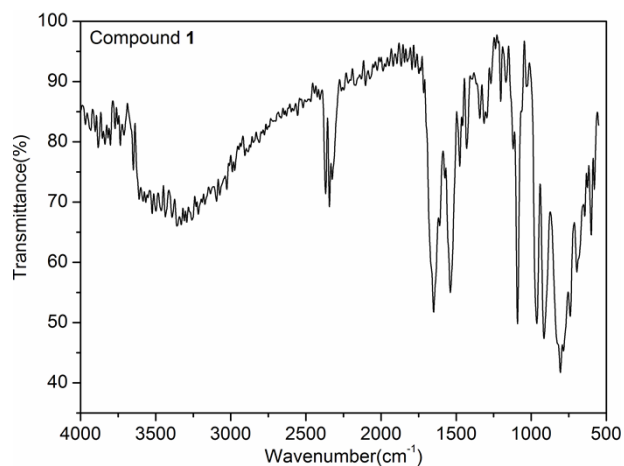


Fig. S3 The IR spectrum of compound 1.

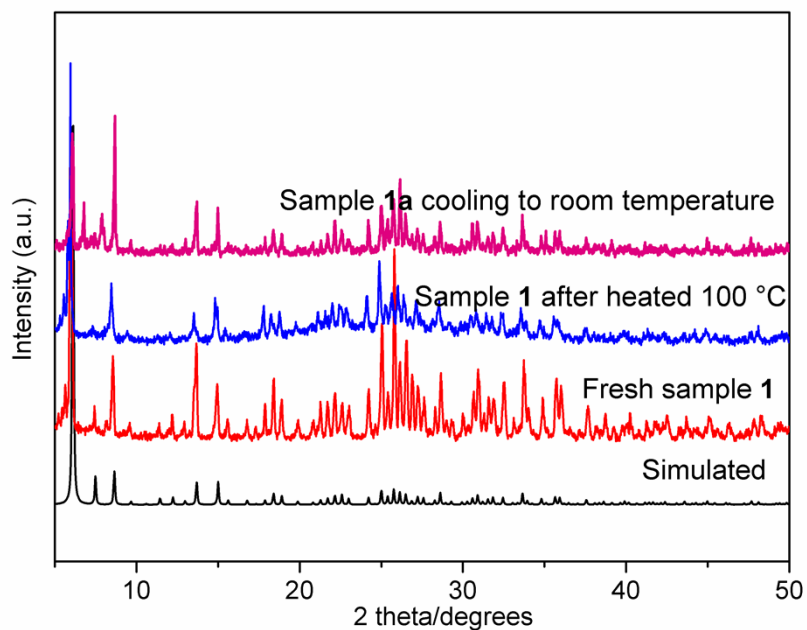
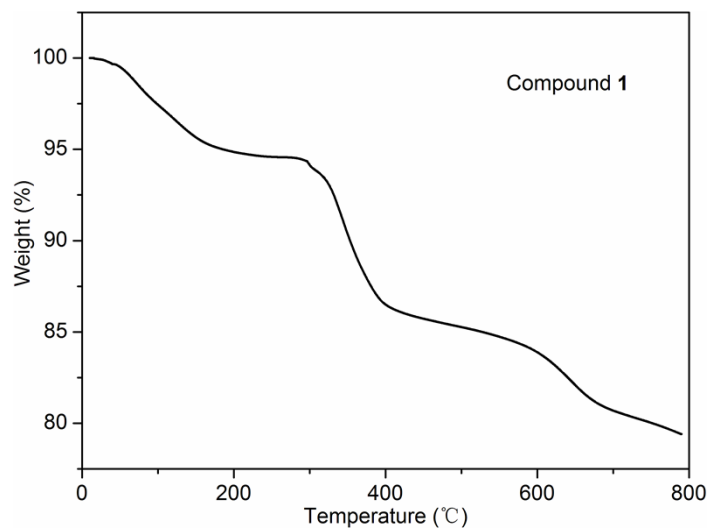


Fig. S4 X-ray powder diffraction patterns of compound **1** (simulated from single-crystal X-ray data and fresh sample), **1a** and **1a** cooling to room temperature



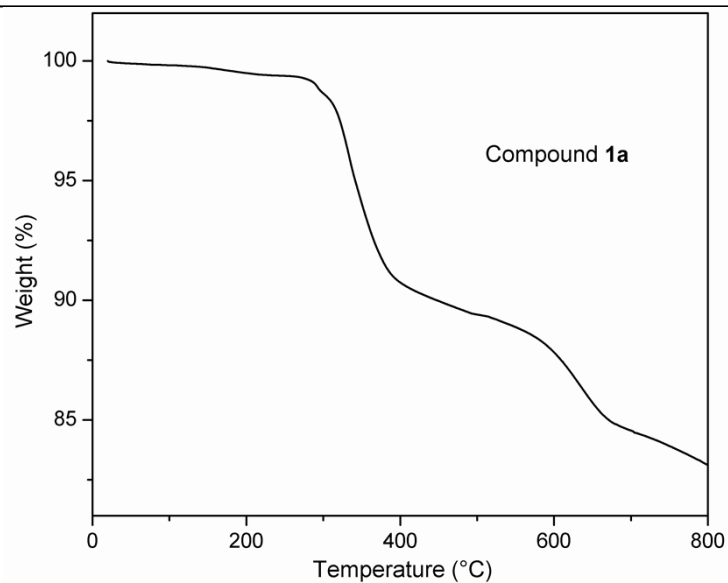


Fig. S5 The TG curves of compounds 1 and 1a.

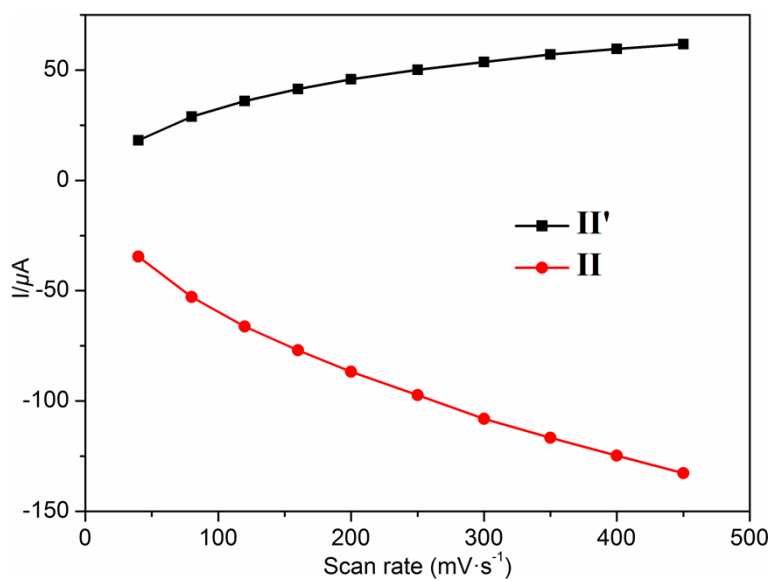


Fig. S6 The plots of the anodic and cathodic peak currents (II-II') against scan rates.