Supporting Information

A {Cu_6}-Added Polyoxometalate Cluster-organic Framework: Synthesis, Structure and Application as a Solid Support for Enzyme Immobilization

Zhao-Min Su,[†a] Yongchun Wang,[†a] Zhikun Xu,[b] Wenhui Shang,[a] Zhiyu Jia,*[a] and Guo-Yu Yang*[a]

[a.] MOE Key Laboratory of Cluster Science, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, China.

[b.] College of Veterinary Medicine, Henan University of Animal Husbandry and Economy, Longzihu North road No 6, Zhengzhou, 450046, Henan, P. R. China.

[†] These authors contributed equally to this work.

E-Mail: jzy@bit.edu.cn, ygy@bit.edu.cn

EXPERIMENTAL SECTION

Materials and Methods

The starting materials $Na_9[A\text{-}\alpha\text{-}PW_9O_{34}]\cdot 7H_2O$ was prepared according to the literatures. All other chemicals employed in this study were analytical reagent without further purification. Elemental analyses of C and H were carried out with a Flash EA1112 elemental analyzer. IR spectra (KBr pellets) were recorded on a Smart Omni-Transmission spectrometer over a range of 400-4000 cm^{-1}. TGA were performed on a Mettler Toledo TGA/DSC 1000 analyzer at air atmosphere with a heating rate of 10 ºC /min. These data can be obtained free of charge from Powder XRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu Kα radiation (λ = 1.54056 Å). UV/Vis-NIR diffuse reflectance spectra were recorded on a UV 3600 spectrophotometer (Shimadzu, Japan).

Synthesis of $\{Cu_{0.5}Na_{0.25}Cl_{0.25}(dap)_{0.5}(H_2O)_{1.5}[Cu_6(\mu\text{-}OH)_3(H_2O)_4(dap)_{2.16}(B\text{-}\alpha\text{-}PW_9O_{34})](1,4\text{-}NDC)_{1/2}\}$ (1):

A sample of $Na_9[A\text{-}\alpha\text{-}PW_9O_{34}]\cdot 7H_2O$ (0.49 g), HAc (0.2mL), $CuCl_2\cdot 2H_2O$ (0.34g) was stirred in distilled water (10 mL) for 5 min, forming a bule clear solution. Then, dap (0.1 mL) was added dropwise with continuous stirring. To this solution, 1,4-H_2NDC (0.20 g) was added and the pH was adjusted to 4.6 with 2 M NaOH. The resulting solution was stirred for 120 min and sealed in a 35 mL stainless steel reactor with a Teflon liner and heated at 80ºC for 5 days, and then cooled to room

temperature, upon which green crystals were obtained. Yields: 36% (220 mg) based on $Na_9[A\text{-}\alpha\text{-}PW_9O_{34}]\cdot 7H_2O$.

Table S1. Crystallographic data and structure refinements for **1**.

	Cu-POMCOF
formula	$Na_{0.4}C_{16.50}H_{55}Cl_{0.6}Cu_{6.6}N_7PO_{46}W_9$
Formula weight	3205.42
Crystal color	blue
crystal system	monoclinic
space group	$P2_1/c$
Temperature	173(2) K
Wavelength	0.71073 Å
a/Å	10.9919(11)
b/Å	20.479(2)
c/Å	27.193(3)
α/°	90
β/°	91.529(3)
γ/°	90
V/Å^3	6119.2(11)
Z	4
D_c/g cm^{-3}	3.479
μ/mm^{-1}	19.188
F_{000}	5800
Crystal size	0.250 x 0.220 x 0.180 mm^3
θ range/°	1.798 to 30.000
Reflections collected	82582
Independent reflections	17725
R(int)	0.0424
Completeness	1.000
Data/restraints/parameters	17725/152/926
Goodness-of-fit on F^2	1.067
Final *R* indices [I>2sigma(I)]	R_1 = 0.0322, wR_2 = 0.0617
R indices (all data)	R_1 = 0.0442, wR_2 = 0.0651
Largest diff. peak and hole/e.Å^{-3}	2.623/-2.752

In asymmetric unit of this data, there were two disordered water molecules which

could not be restrained properly. Therefore, SQUEEZE algorithm was used to omit them. The moiety including Cu7 was strongly disordered and we have to divide it into three parts (50% Cu^{2+} and 25% Na^{+}). 19 ISOR, 1 SIMU and 20 DFIX instructions were used to restrain disordered moiety, naphthalenedicarboxylate ligand and hydroxide anions so that there were 152 restraints in the data. Hydrogen of water molecules could not be found and others were put in calculated positions.

Table S2. Elemental analysis for Cu-POMCOF.

Elemental analysis		calcd (%)	Found (%)
Compound **1**	C	6.77	7.28
	N	3.51	2.89
	H	1.25	1.74

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon_sq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	3496(1)	6512(1)	7130(1)	9(1)
W(1)	1033(1)	7534(1)	7523(1)	18(1)
W(2)	3124(1)	8107(1)	6554(1)	19(1)
W(3)	925(1)	6762(1)	6293(1)	23(1)
W(4)	3504(1)	7272(1)	8305(1)	14(1)
W(5)	5592(1)	7795(1)	7331(1)	13(1)
W(6)	5488(1)	7099(1)	6208(1)	18(1)
W(7)	3274(1)	5762(1)	5939(1)	20(1)
W(8)	1386(1)	5242(1)	6824(1)	20(1)
W(9)	1547(1)	6028(1)	8059(1)	18(1)
Cu(1)	4673(1)	5641(1)	8020(1)	12(1)
Cu(2)	4553(1)	4951(1)	6973(1)	13(1)
Cu(3)	6456(1)	6134(1)	7223(1)	11(1)
Cu(4)	6499(1)	6648(1)	8344(1)	17(1)
Cu(5)	2985(1)	4427(1)	7767(1)	18(1)
Cu(6)	6289(1)	5379(1)	6225(1)	19(1)
O(1)	2077(4)	8021(2)	7105(2)	20(1)
O(2)	2006(4)	7474(2)	6264(2)	24(1)
O(3)	546(4)	7083(2)	6931(2)	22(1)
O(4)	-156(4)	8057(2)	7606(2)	32(1)
O(5)	2622(5)	8826(2)	6291(2)	33(1)
O(6)	-295(5)	7015(3)	5946(2)	37(1)
O(7)	2070(4)	7789(2)	8056(2)	19(1)
O(8)	4365(4)	8391(2)	6984(2)	18(1)
O(9)	4260(5)	7815(2)	6098(2)	24(1)
O(10)	1866(5)	6327(2)	5812(2)	26(1)
O(11)	392(4)	5925(2)	6507(2)	24(1)
O(12)	531(4)	6796(2)	7876(2)	22(1)
O(13)	4437(4)	7790(2)	7845(2)	15(1)

O(14)	6158(4)	7718(2)	6667(2)	18(1)
O(15)	4257(4)	6531(2)	5933(2)	21(1)
O(16)	2098(4)	5165(2)	6195(2)	22(1)
O(17)	1022(4)	5653(2)	7441(2)	19(1)
O(18)	2321(4)	6660(2)	8508(2)	19(1)
O(19)	3788(5)	7693(2)	8840(2)	25(1)
O(20)	6595(4)	8376(2)	7557(2)	20(1)
O(21)	6358(5)	7216(2)	5700(2)	30(1)
O(22)	3484(5)	5473(3)	5355(2)	31(1)
O(23)	334(5)	4619(2)	6816(2)	35(1)
O(24)	568(5)	5630(2)	8447(2)	32(1)
O(25)	4699(4)	6670(2)	8298(2)	17(1)
O(26)	6306(4)	7040(2)	7496(2)	14(1)
O(27)	6232(4)	6438(2)	6537(2)	17(1)
O(28)	4473(4)	5337(2)	6311(2)	15(1)
O(29)	2761(4)	4861(2)	7099(2)	16(1)
O(30)	2903(4)	5537(2)	8081(2)	15(1)
O(31)	2712(4)	6755(2)	7557(2)	13(1)
O(32)	4139(4)	7113(2)	6907(2)	13(1)
O(33)	2652(4)	6207(2)	6731(2)	16(1)
O(34)	4400(4)	6013(2)	7321(2)	12(1)
O(35)	6390(4)	5853(2)	7915(2)	15(1)
O(36)	4664(4)	4668(2)	7649(2)	15(1)
O(37)	6301(4)	5235(2)	6939(2)	14(1)
O(38)	4926(5)	5277(2)	8684(2)	26(1)
O(39)	6269(6)	5986(3)	9019(2)	44(2)
O(40)	4945(7)	3968(3)	6620(2)	46(2)
O(41)	8510(5)	6192(3)	7244(2)	41(2)
C(1)	6059(19)	5094(14)	9860(10)	32(4)
C(2)	5118(16)	5298(12)	9539(7)	26(3)
C(3)	3885(17)	5268(17)	9695(11)	35(4)
C(4)	2912(12)	5512(8)	9397(5)	30(3)
C(5)	1742(14)	5487(9)	9569(6)	39(4)
C(1')	3632(17)	5027(14)	10177(10)	32(4)
C(2')	4600(18)	4792(12)	10474(8)	26(3)
C(3')	5810(20)	4837(16)	10320(12)	35(4)
C(4')	2420(14)	5005(9)	10333(6)	42(4)
C(5')	1483(17)	5268(12)	10038(7)	56(6)

C(6)	5518(8)	5526(4)	9040(3)	31(2)
N(1)	6645(6)	7530(3)	8660(3)	36(2)
N(2)	8298(5)	6620(4)	8418(2)	32(2)
C(7)	8216(15)	8377(8)	8889(8)	131(8)
C(8)	7962(10)	7745(6)	8622(6)	79(4)
C(9)	8716(9)	7168(6)	8724(5)	73(4)
N(3)	3263(7)	4146(3)	8469(2)	34(2)
N(4)	1266(6)	4185(3)	7875(3)	36(2)
C(10)	1973(13)	3730(7)	9164(5)	43(3)
C(11)	2070(11)	4108(4)	8701(4)	59(3)
C(12)	1224(10)	3800(4)	8342(4)	58(3)
N(3')	1266(6)	4185(3)	7875(3)	36(2)
N(4')	3263(7)	4146(3)	8469(2)	34(2)
C(10')	180(19)	3753(13)	8680(9)	42(6)
C(11')	1224(10)	3800(4)	8342(4)	58(3)
C(12')	2070(11)	4108(4)	8701(4)	59(3)
N(5)	8062(6)	5228(4)	6164(3)	45(2)
N(6)	6305(7)	5569(4)	5511(2)	38(2)
C(13)	9582(17)	5132(17)	5447(9)	95(10)
C(14)	8360(10)	5230(8)	5635(5)	80(4)
C(15)	7567(11)	5715(6)	5389(5)	77(4)
N(5')	6305(7)	5569(4)	5511(2)	38(2)
N(6')	8062(6)	5228(4)	6164(3)	45(2)
C(13')	7950(30)	5970(13)	4913(7)	82(8)
C(14')	7567(11)	5715(6)	5389(5)	77(4)
C(15')	8360(10)	5230(8)	5635(5)	80(4)
C(16)	1230(30)	6731(14)	10057(16)	168(13)
C(17)	2050(20)	7329(12)	10065(11)	107(6)
C(18)	1350(20)	7856(11)	9786(11)	97(7)
N(7)	3260(20)	7150(13)	9936(10)	112(7)
N(8)	2294(17)	8340(9)	9701(7)	61(5)
Cl(1A)	4849(9)	8883(4)	9505(2)	15(3)
O(42A)	4849(9)	8883(4)	9505(2)	15(3)
Cu(7)	3936(3)	7927(2)	9637(1)	38(1)
O(43)	5990(40)	7100(20)	9719(16)	87(12)
Cu(7')	3666(9)	8399(5)	9554(3)	36(2)
O(42)	3750(20)	9153(9)	9143(9)	34(5)
O(43A)	5470(20)	7459(12)	9750(7)	66(6)

Cl(1)	5426(16)	8715(6)	9510(4)	34(4)
Na(1)	4514(14)	7735(7)	9715(5)	37(3)
O(43B)	6630(30)	6950(20)	9707(11)	82(11)
O(47)	2240(16)	7991(9)	9520(6)	69(5)
O(44)	8190(6)	46(3)	3208(3)	56(2)
O(45)	2134(7)	5713(3)	2708(3)	66(2)
O(46)	1322(8)	8704(4)	8752(4)	82(3)

Table S4. Bond lengths [Å] and angles [°] for platon_sq.

P(1)-O(34)	1.509(4)
P(1)-O(33)	1.541(4)
P(1)-O(31)	1.546(4)
P(1)-O(32)	1.551(4)
W(1)-O(4)	1.709(5)
W(1)-O(12)	1.880(5)
W(1)-O(7)	1.893(5)
W(1)-O(1)	1.916(5)
W(1)-O(3)	1.920(5)
W(1)-O(31)	2.438(4)
W(2)-O(5)	1.722(5)
W(2)-O(8)	1.865(5)
W(2)-O(9)	1.881(5)
W(2)-O(1)	1.920(5)
W(2)-O(2)	1.940(5)
W(2)-O(32)	2.500(4)
W(3)-O(6)	1.702(5)
W(3)-O(2)	1.884(5)
W(3)-O(11)	1.906(5)
W(3)-O(10)	1.910(5)
W(3)-O(3)	1.911(5)
W(3)-O(33)	2.488(4)
W(4)-O(19)	1.714(5)
W(4)-O(25)	1.802(4)
W(4)-O(18)	1.898(4)
W(4)-O(13)	1.951(4)
W(4)-O(7)	2.002(4)
W(4)-O(31)	2.433(4)
W(5)-O(20)	1.724(4)
W(5)-O(26)	1.786(4)
W(5)-O(13)	1.913(4)
W(5)-O(14)	1.933(4)
W(5)-O(8)	2.034(4)
W(5)-O(32)	2.393(4)
W(6)-O(21)	1.717(5)
W(6)-O(27)	1.808(4)

W(6)-O(14)	1.912(4)
W(6)-O(15)	1.921(5)
W(6)-O(9)	2.009(5)
W(6)-O(32)	2.443(4)
W(7)-O(22)	1.716(5)
W(7)-O(28)	1.856(4)
W(7)-O(15)	1.910(5)
W(7)-O(16)	1.922(5)
W(7)-O(10)	1.956(5)
W(7)-O(33)	2.452(5)
W(8)-O(23)	1.721(5)
W(8)-O(29)	1.840(4)
W(8)-O(16)	1.908(5)
W(8)-O(17)	1.928(5)
W(8)-O(11)	1.962(4)
W(8)-O(33)	2.435(4)
W(9)-O(24)	1.731(5)
W(9)-O(30)	1.797(4)
W(9)-O(17)	1.921(5)
W(9)-O(18)	1.960(5)
W(9)-O(12)	1.984(4)
W(9)-O(31)	2.411(4)
Cu(1)-O(35)	1.964(4)
Cu(1)-O(38)	1.967(5)
Cu(1)-O(30)	1.969(4)
Cu(1)-O(34)	2.061(4)
Cu(1)-O(36)	2.234(4)
Cu(1)-O(25)	2.239(4)
Cu(1)-Cu(4)	2.9925(11)
Cu(2)-O(36)	1.930(4)
Cu(2)-O(28)	1.965(4)
Cu(2)-O(37)	2.012(4)
Cu(2)-O(29)	2.016(4)
Cu(2)-O(40)	2.274(6)
Cu(2)-O(34)	2.380(4)
Cu(2)-Cu(6)	2.9579(11)
Cu(2)-Cu(5)	2.9981(11)
Cu(3)-O(35)	1.971(4)

Cu(3)-O(27)	1.975(4)
Cu(3)-O(37)	2.003(4)
Cu(3)-O(26)	2.005(4)
Cu(3)-O(41)	2.260(5)
Cu(3)-O(34)	2.296(4)
Cu(4)-O(25)	1.979(4)
Cu(4)-N(2)	1.983(6)
Cu(4)-O(35)	2.005(4)
Cu(4)-N(1)	2.006(6)
Cu(4)-O(39)	2.301(6)
Cu(5)-O(36)	1.946(4)
Cu(5)-N(3')	1.982(6)
Cu(5)-N(4)	1.982(6)
Cu(5)-N(4')	2.008(6)
Cu(5)-N(3)	2.008(6)
Cu(5)-O(29)	2.033(5)
Cu(5)-O(20)#1	2.375(4)
Cu(5)-O(30)	2.432(4)
Cu(6)-O(37)	1.963(4)
Cu(6)-N(5')	1.980(7)
Cu(6)-N(6)	1.980(7)
Cu(6)-N(6')	1.985(7)
Cu(6)-N(5)	1.985(7)
Cu(6)-O(28)	2.018(4)
Cu(6)-O(27)	2.330(4)
O(19)-Cu(7)	2.222(6)
O(19)-Cu(7')	2.426(11)
O(19)-Na(1)	2.492(16)
O(35)-H(35)	0.840(6)
O(36)-H(36)	0.840(6)
O(37)-H(37)	0.840(6)
O(38)-C(6)	1.261(9)
O(39)-C(6)	1.254(10)
C(1)-C(3')	1.39(4)
C(1)-C(2)	1.399(18)
C(1)-H(1)	0.9500
C(2)-C(3)	1.432(18)
C(2)-C(6)	1.513(16)

C(3)-C(4)	1.415(17)
C(3)-C(1')	1.43(4)
C(4)-C(5)	1.381(15)
C(4)-H(4)	0.9500
C(5)-C(5')	1.39(2)
C(5)-H(5)	0.9500
C(1')-C(2')	1.40(3)
C(1')-C(4')	1.409(17)
C(2')-C(3')	1.40(3)
C(3')-H(3')	0.9500
C(4')-C(5')	1.396(16)
C(4')-H(4')	0.9500
C(5')-H(5')	0.9500
N(1)-C(8)	1.519(13)
N(1)-H(1A)	0.9100
N(1)-H(1B)	0.9100
N(2)-C(9)	1.464(11)
N(2)-H(2A)	0.9100
N(2)-H(2B)	0.9100
C(7)-C(8)	1.506(16)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(9)	1.466(16)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
N(3)-C(11)	1.472(12)
N(3)-H(3A)	0.9100
N(3)-H(3B)	0.9100
N(4)-C(12)	1.497(12)
N(4)-H(4A)	0.9100
N(4)-H(4B)	0.9100
C(10)-C(11)	1.485(15)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.473(16)

C(11)-H(11)	1.0000
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
N(3')-C(11')	1.497(12)
N(3')-H(3'A)	0.9100
N(3')-H(3'B)	0.9100
N(4')-C(12')	1.472(12)
N(4')-H(4'A)	0.9100
N(4')-H(4'B)	0.9100
C(10')-C(11')	1.493(16)
C(10')-H(10D)	0.9800
C(10')-H(10E)	0.9800
C(10')-H(10F)	0.9800
C(11')-C(12')	1.473(16)
C(11')-H(11')	1.0000
C(12')-H(12C)	0.9900
C(12')-H(12D)	0.9900
N(5)-C(14)	1.484(14)
N(5)-H(5A)	0.9100
N(5)-H(5B)	0.9100
N(6)-C(15)	1.466(13)
N(6)-H(6A)	0.9100
N(6)-H(6B)	0.9100
C(13)-C(14)	1.464(16)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.470(17)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
N(5')-C(14')	1.466(13)
N(5')-H(5'A)	0.9100
N(5')-H(5'B)	0.9100
N(6')-C(15')	1.484(14)
N(6')-H(6'A)	0.9100
N(6')-H(6'B)	0.9100
C(13')-C(14')	1.469(15)

C(13')-H(13D)	0.9800
C(13')-H(13E)	0.9800
C(13')-H(13F)	0.9800
C(14')-C(15')	1.470(17)
C(14')-H(14')	1.0000
C(15')-H(15C)	0.9900
C(15')-H(15D)	0.9900
C(16)-C(17)	1.523(18)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-N(7)	1.432(17)
C(17)-C(18)	1.520(17)
C(17)-H(17)	1.0000
C(18)-N(8)	1.460(17)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
N(7)-Cu(7)	1.94(2)
N(7)-H(7D)	0.9100
N(7)-H(7E)	0.9100
N(8)-Cu(7)	2.00(2)
N(8)-H(8A)	0.9100
N(8)-H(8B)	0.9100
Cl(1A)-Cu(7)	2.234(7)
Cu(7)-O(43)	2.82(4)
Cu(7')-O(42)	1.91(2)
Cu(7')-O(43A)	2.80(3)
Cl(1)-Na(1)	2.318(19)
Na(1)-O(47)	2.59(2)
Na(1)-O(43B)	2.83(5)
O(34)-P(1)-O(33)	110.2(2)
O(34)-P(1)-O(31)	109.6(2)
O(33)-P(1)-O(31)	108.8(2)
O(34)-P(1)-O(32)	111.7(2)
O(33)-P(1)-O(32)	108.6(2)
O(31)-P(1)-O(32)	107.9(2)
O(4)-W(1)-O(12)	101.5(2)
O(4)-W(1)-O(7)	99.9(2)

O(12)-W(1)-O(7)	90.5(2)
O(4)-W(1)-O(1)	103.0(2)
O(12)-W(1)-O(1)	155.38(18)
O(7)-W(1)-O(1)	87.3(2)
O(4)-W(1)-O(3)	102.5(2)
O(12)-W(1)-O(3)	87.9(2)
O(7)-W(1)-O(3)	157.45(19)
O(1)-W(1)-O(3)	84.9(2)
O(4)-W(1)-O(31)	170.0(2)
O(12)-W(1)-O(31)	71.79(16)
O(7)-W(1)-O(31)	73.26(16)
O(1)-W(1)-O(31)	84.15(16)
O(3)-W(1)-O(31)	84.90(16)
O(5)-W(2)-O(8)	102.4(2)
O(5)-W(2)-O(9)	102.0(2)
O(8)-W(2)-O(9)	91.4(2)
O(5)-W(2)-O(1)	102.2(2)
O(8)-W(2)-O(1)	89.1(2)
O(9)-W(2)-O(1)	155.04(18)
O(5)-W(2)-O(2)	102.1(2)
O(8)-W(2)-O(2)	155.25(18)
O(9)-W(2)-O(2)	86.7(2)
O(1)-W(2)-O(2)	82.5(2)
O(5)-W(2)-O(32)	172.1(2)
O(8)-W(2)-O(32)	72.66(16)
O(9)-W(2)-O(32)	72.33(17)
O(1)-W(2)-O(32)	84.06(16)
O(2)-W(2)-O(32)	83.31(16)
O(6)-W(3)-O(2)	103.2(2)
O(6)-W(3)-O(11)	101.5(2)
O(2)-W(3)-O(11)	155.20(19)
O(6)-W(3)-O(10)	101.2(2)
O(2)-W(3)-O(10)	88.8(2)
O(11)-W(3)-O(10)	88.1(2)
O(6)-W(3)-O(3)	102.2(2)
O(2)-W(3)-O(3)	85.6(2)
O(11)-W(3)-O(3)	87.5(2)
O(10)-W(3)-O(3)	156.62(19)

O(6)-W(3)-O(33)	170.2(2)
O(2)-W(3)-O(33)	84.24(17)
O(11)-W(3)-O(33)	71.39(16)
O(10)-W(3)-O(33)	72.29(17)
O(3)-W(3)-O(33)	84.55(17)
O(19)-W(4)-O(25)	103.7(2)
O(19)-W(4)-O(18)	101.3(2)
O(25)-W(4)-O(18)	93.28(19)
O(19)-W(4)-O(13)	100.6(2)
O(25)-W(4)-O(13)	88.26(19)
O(18)-W(4)-O(13)	157.06(19)
O(19)-W(4)-O(7)	98.3(2)
O(25)-W(4)-O(7)	157.84(19)
O(18)-W(4)-O(7)	84.69(19)
O(13)-W(4)-O(7)	85.34(18)
O(19)-W(4)-O(31)	169.09(19)
O(25)-W(4)-O(31)	86.51(17)
O(18)-W(4)-O(31)	73.98(17)
O(13)-W(4)-O(31)	83.29(16)
O(7)-W(4)-O(31)	71.70(16)
O(20)-W(5)-O(26)	103.7(2)
O(20)-W(5)-O(13)	100.0(2)
O(26)-W(5)-O(13)	96.21(19)
O(20)-W(5)-O(14)	99.8(2)
O(26)-W(5)-O(14)	90.74(19)
O(13)-W(5)-O(14)	156.76(19)
O(20)-W(5)-O(8)	99.23(19)
O(26)-W(5)-O(8)	156.65(18)
O(13)-W(5)-O(8)	84.14(18)
O(14)-W(5)-O(8)	80.84(19)
O(20)-W(5)-O(32)	170.38(18)
O(26)-W(5)-O(32)	84.20(16)
O(13)-W(5)-O(32)	84.37(16)
O(14)-W(5)-O(32)	74.28(16)
O(8)-W(5)-O(32)	72.58(16)
O(21)-W(6)-O(27)	104.4(2)
O(21)-W(6)-O(14)	102.7(2)
O(27)-W(6)-O(14)	90.66(19)

O(21)-W(6)-O(15)	100.0(2)
O(27)-W(6)-O(15)	92.46(19)
O(14)-W(6)-O(15)	155.5(2)
O(21)-W(6)-O(9)	99.5(2)
O(27)-W(6)-O(9)	155.9(2)
O(14)-W(6)-O(9)	81.91(19)
O(15)-W(6)-O(9)	85.4(2)
O(21)-W(6)-O(32)	170.8(2)
O(27)-W(6)-O(32)	84.19(17)
O(14)-W(6)-O(32)	73.41(16)
O(15)-W(6)-O(32)	82.74(17)
O(9)-W(6)-O(32)	71.77(17)
O(22)-W(7)-O(28)	103.4(2)
O(22)-W(7)-O(15)	100.7(2)
O(28)-W(7)-O(15)	89.89(19)
O(22)-W(7)-O(16)	103.0(2)
O(28)-W(7)-O(16)	88.82(18)
O(15)-W(7)-O(16)	156.0(2)
O(22)-W(7)-O(10)	99.5(2)
O(28)-W(7)-O(10)	157.1(2)
O(15)-W(7)-O(10)	87.5(2)
O(16)-W(7)-O(10)	84.5(2)
O(22)-W(7)-O(33)	171.2(2)
O(28)-W(7)-O(33)	84.66(16)
O(15)-W(7)-O(33)	82.64(17)
O(16)-W(7)-O(33)	73.35(17)
O(10)-W(7)-O(33)	72.44(17)
O(23)-W(8)-O(29)	103.6(2)
O(23)-W(8)-O(16)	102.6(2)
O(29)-W(8)-O(16)	88.66(19)
O(23)-W(8)-O(17)	100.4(2)
O(29)-W(8)-O(17)	91.16(19)
O(16)-W(8)-O(17)	156.36(18)
O(23)-W(8)-O(11)	99.0(2)
O(29)-W(8)-O(11)	157.25(19)
O(16)-W(8)-O(11)	84.3(2)
O(17)-W(8)-O(11)	86.8(2)
O(23)-W(8)-O(33)	170.3(2)

O(29)-W(8)-O(33)	85.46(16)
O(16)-W(8)-O(33)	74.00(17)
O(17)-W(8)-O(33)	82.41(17)
O(11)-W(8)-O(33)	71.81(16)
O(24)-W(9)-O(30)	104.2(2)
O(24)-W(9)-O(17)	99.7(2)
O(30)-W(9)-O(17)	92.03(19)
O(24)-W(9)-O(18)	101.4(2)
O(30)-W(9)-O(18)	90.14(19)
O(17)-W(9)-O(18)	157.62(19)
O(24)-W(9)-O(12)	99.9(2)
O(30)-W(9)-O(12)	155.80(19)
O(17)-W(9)-O(12)	86.77(19)
O(18)-W(9)-O(12)	82.23(19)
O(24)-W(9)-O(31)	169.74(18)
O(30)-W(9)-O(31)	84.95(16)
O(17)-W(9)-O(31)	84.47(17)
O(18)-W(9)-O(31)	73.53(16)
O(12)-W(9)-O(31)	70.87(16)
O(35)-Cu(1)-O(38)	96.0(2)
O(35)-Cu(1)-O(30)	172.53(17)
O(38)-Cu(1)-O(30)	89.8(2)
O(35)-Cu(1)-O(34)	84.36(17)
O(38)-Cu(1)-O(34)	179.31(19)
O(30)-Cu(1)-O(34)	89.85(17)
O(35)-Cu(1)-O(36)	97.12(17)
O(38)-Cu(1)-O(36)	94.24(18)
O(30)-Cu(1)-O(36)	87.06(17)
O(34)-Cu(1)-O(36)	85.12(16)
O(35)-Cu(1)-O(25)	80.69(17)
O(38)-Cu(1)-O(25)	92.65(18)
O(30)-Cu(1)-O(25)	94.42(17)
O(34)-Cu(1)-O(25)	87.99(16)
O(36)-Cu(1)-O(25)	172.96(16)
O(35)-Cu(1)-Cu(4)	41.58(12)
O(38)-Cu(1)-Cu(4)	85.05(15)
O(30)-Cu(1)-Cu(4)	134.92(13)
O(34)-Cu(1)-Cu(4)	95.61(12)

O(36)-Cu(1)-Cu(4)	137.94(11)
O(25)-Cu(1)-Cu(4)	41.41(11)
O(36)-Cu(2)-O(28)	173.69(18)
O(36)-Cu(2)-O(37)	95.40(18)
O(28)-Cu(2)-O(37)	82.03(18)
O(36)-Cu(2)-O(29)	81.26(18)
O(28)-Cu(2)-O(29)	99.91(18)
O(37)-Cu(2)-O(29)	166.48(17)
O(36)-Cu(2)-O(40)	97.37(19)
O(28)-Cu(2)-O(40)	88.53(19)
O(37)-Cu(2)-O(40)	92.6(2)
O(29)-Cu(2)-O(40)	100.9(2)
O(36)-Cu(2)-O(34)	84.16(16)
O(28)-Cu(2)-O(34)	89.72(16)
O(37)-Cu(2)-O(34)	80.30(15)
O(29)-Cu(2)-O(34)	86.31(15)
O(40)-Cu(2)-O(34)	172.8(2)
O(36)-Cu(2)-Cu(6)	135.94(13)
O(28)-Cu(2)-Cu(6)	42.73(12)
O(37)-Cu(2)-Cu(6)	41.28(13)
O(29)-Cu(2)-Cu(6)	142.63(13)
O(40)-Cu(2)-Cu(6)	80.76(17)
O(34)-Cu(2)-Cu(6)	93.23(10)
O(36)-Cu(2)-Cu(5)	39.51(13)
O(28)-Cu(2)-Cu(5)	142.30(13)
O(37)-Cu(2)-Cu(5)	134.79(13)
O(29)-Cu(2)-Cu(5)	42.44(13)
O(40)-Cu(2)-Cu(5)	96.10(17)
O(34)-Cu(2)-Cu(5)	89.55(10)
Cu(6)-Cu(2)-Cu(5)	174.35(3)
O(35)-Cu(3)-O(27)	170.65(18)
O(35)-Cu(3)-O(37)	95.39(18)
O(27)-Cu(3)-O(37)	85.30(18)
O(35)-Cu(3)-O(26)	84.95(17)
O(27)-Cu(3)-O(26)	92.83(17)
O(37)-Cu(3)-O(26)	170.41(17)
O(35)-Cu(3)-O(41)	93.1(2)
O(27)-Cu(3)-O(41)	96.1(2)

O(37)-Cu(3)-O(41)	97.58(19)
O(26)-Cu(3)-O(41)	91.98(19)
O(35)-Cu(3)-O(34)	78.23(16)
O(27)-Cu(3)-O(34)	92.64(16)
O(37)-Cu(3)-O(34)	82.60(15)
O(26)-Cu(3)-O(34)	88.09(16)
O(41)-Cu(3)-O(34)	171.2(2)
O(25)-Cu(4)-N(2)	177.7(2)
O(25)-Cu(4)-O(35)	86.46(18)
N(2)-Cu(4)-O(35)	94.6(2)
O(25)-Cu(4)-N(1)	94.3(2)
N(2)-Cu(4)-N(1)	85.1(3)
O(35)-Cu(4)-N(1)	169.8(3)
O(25)-Cu(4)-O(39)	86.1(2)
N(2)-Cu(4)-O(39)	91.8(3)
O(35)-Cu(4)-O(39)	88.9(2)
N(1)-Cu(4)-O(39)	101.4(3)
O(25)-Cu(4)-Cu(1)	48.42(13)
N(2)-Cu(4)-Cu(1)	132.0(2)
O(35)-Cu(4)-Cu(1)	40.55(13)
N(1)-Cu(4)-Cu(1)	142.36(19)
O(39)-Cu(4)-Cu(1)	75.07(14)
O(36)-Cu(5)-N(3')	179.0(3)
O(36)-Cu(5)-N(4)	179.0(3)
O(36)-Cu(5)-N(4')	96.2(3)
N(3')-Cu(5)-N(4')	84.8(3)
O(36)-Cu(5)-N(3)	96.2(3)
N(4)-Cu(5)-N(3)	84.8(3)
O(36)-Cu(5)-O(29)	80.47(18)
N(3')-Cu(5)-O(29)	98.5(3)
N(4)-Cu(5)-O(29)	98.5(3)
N(4')-Cu(5)-O(29)	170.6(2)
N(3)-Cu(5)-O(29)	170.6(2)
O(36)-Cu(5)-O(20)#1	88.50(17)
N(4)-Cu(5)-O(20)#1	91.4(2)
N(3)-Cu(5)-O(20)#1	93.8(2)
O(29)-Cu(5)-O(20)#1	94.90(17)
O(36)-Cu(5)-O(30)	82.22(16)

N(3')-Cu(5)-O(30)	97.9(2)
N(4)-Cu(5)-O(30)	97.9(2)
N(4')-Cu(5)-O(30)	86.6(2)
N(3)-Cu(5)-O(30)	86.6(2)
O(29)-Cu(5)-O(30)	84.22(16)
O(20)#1-Cu(5)-O(30)	170.70(15)
O(36)-Cu(5)-Cu(2)	39.15(13)
N(3')-Cu(5)-Cu(2)	139.9(2)
N(4)-Cu(5)-Cu(2)	139.9(2)
N(4')-Cu(5)-Cu(2)	135.3(2)
N(3)-Cu(5)-Cu(2)	135.3(2)
O(29)-Cu(5)-Cu(2)	42.01(12)
O(20)#1-Cu(5)-Cu(2)	86.32(12)
O(30)-Cu(5)-Cu(2)	86.86(10)
O(37)-Cu(6)-N(5')	177.2(3)
O(37)-Cu(6)-N(6)	177.2(3)
O(37)-Cu(6)-N(6')	94.5(3)
N(5')-Cu(6)-N(6')	85.1(3)
O(37)-Cu(6)-N(5)	94.5(3)
N(6)-Cu(6)-N(5)	85.1(3)
O(37)-Cu(6)-O(28)	81.93(17)
N(5')-Cu(6)-O(28)	99.0(3)
N(6)-Cu(6)-O(28)	99.0(3)
N(6')-Cu(6)-O(28)	168.4(3)
N(5)-Cu(6)-O(28)	168.4(3)
O(37)-Cu(6)-O(27)	77.25(17)
N(5')-Cu(6)-O(27)	100.1(2)
N(6)-Cu(6)-O(27)	100.1(2)
N(6')-Cu(6)-O(27)	102.2(3)
N(5)-Cu(6)-O(27)	102.2(3)
O(28)-Cu(6)-O(27)	87.80(16)
O(37)-Cu(6)-Cu(2)	42.56(12)
N(5')-Cu(6)-Cu(2)	139.0(2)
N(6)-Cu(6)-Cu(2)	139.0(2)
N(6')-Cu(6)-Cu(2)	131.6(2)
N(5)-Cu(6)-Cu(2)	131.6(2)
O(28)-Cu(6)-Cu(2)	41.35(12)
O(27)-Cu(6)-Cu(2)	90.10(11)

W(1)-O(1)-W(2)	153.0(3)
W(3)-O(2)-W(2)	153.3(3)
W(3)-O(3)-W(1)	149.8(3)
W(1)-O(7)-W(4)	124.4(2)
W(2)-O(8)-W(5)	124.6(2)
W(2)-O(9)-W(6)	126.1(2)
W(3)-O(10)-W(7)	126.4(2)
W(3)-O(11)-W(8)	127.1(2)
W(1)-O(12)-W(9)	126.4(2)
W(5)-O(13)-W(4)	147.3(2)
W(6)-O(14)-W(5)	122.5(2)
W(7)-O(15)-W(6)	152.8(3)
W(8)-O(16)-W(7)	124.6(2)
W(9)-O(17)-W(8)	150.5(2)
W(4)-O(18)-W(9)	122.9(2)
W(4)-O(19)-Cu(7)	160.8(3)
W(4)-O(19)-Cu(7')	165.2(4)
W(4)-O(19)-Na(1)	151.1(4)
W(5)-O(20)-Cu(5)#2	128.5(2)
W(4)-O(25)-Cu(4)	138.0(2)
W(4)-O(25)-Cu(1)	130.1(2)
Cu(4)-O(25)-Cu(1)	90.17(17)
W(5)-O(26)-Cu(3)	138.4(2)
W(6)-O(27)-Cu(3)	138.3(2)
W(6)-O(27)-Cu(6)	122.2(2)
Cu(3)-O(27)-Cu(6)	92.71(17)
W(7)-O(28)-Cu(2)	134.5(2)
W(7)-O(28)-Cu(6)	127.4(2)
Cu(2)-O(28)-Cu(6)	95.92(18)
W(8)-O(29)-Cu(2)	133.5(2)
W(8)-O(29)-Cu(5)	128.7(2)
Cu(2)-O(29)-Cu(5)	95.54(18)
W(9)-O(30)-Cu(1)	139.2(2)
W(9)-O(30)-Cu(5)	123.3(2)
Cu(1)-O(30)-Cu(5)	91.47(15)
P(1)-O(31)-W(9)	122.7(2)
P(1)-O(31)-W(4)	125.0(2)
W(9)-O(31)-W(4)	88.80(14)

P(1)-O(31)-W(1)	128.2(2)
W(9)-O(31)-W(1)	90.71(14)
W(4)-O(31)-W(1)	90.06(13)
P(1)-O(32)-W(5)	125.4(2)
P(1)-O(32)-W(6)	126.0(2)
W(5)-O(32)-W(6)	88.36(13)
P(1)-O(32)-W(2)	126.3(2)
W(5)-O(32)-W(2)	89.76(13)
W(6)-O(32)-W(2)	89.14(13)
P(1)-O(33)-W(8)	126.2(2)
P(1)-O(33)-W(7)	126.3(2)
W(8)-O(33)-W(7)	87.86(13)
P(1)-O(33)-W(3)	126.1(2)
W(8)-O(33)-W(3)	89.41(13)
W(7)-O(33)-W(3)	88.65(14)
P(1)-O(34)-Cu(1)	130.2(2)
P(1)-O(34)-Cu(3)	121.8(2)
Cu(1)-O(34)-Cu(3)	91.58(15)
P(1)-O(34)-Cu(2)	122.4(2)
Cu(1)-O(34)-Cu(2)	91.14(14)
Cu(3)-O(34)-Cu(2)	88.44(13)
Cu(1)-O(35)-Cu(3)	105.25(19)
Cu(1)-O(35)-Cu(4)	97.87(19)
Cu(3)-O(35)-Cu(4)	108.4(2)
Cu(1)-O(35)-H(35)	119(5)
Cu(3)-O(35)-H(35)	109(5)
Cu(4)-O(35)-H(35)	116(5)
Cu(2)-O(36)-Cu(5)	101.3(2)
Cu(2)-O(36)-Cu(1)	99.26(17)
Cu(5)-O(36)-Cu(1)	98.35(18)
Cu(2)-O(36)-H(36)	116(5)
Cu(5)-O(36)-H(36)	110(5)
Cu(1)-O(36)-H(36)	128(5)
Cu(6)-O(37)-Cu(3)	103.97(19)
Cu(6)-O(37)-Cu(2)	96.17(18)
Cu(3)-O(37)-Cu(2)	108.65(19)
Cu(6)-O(37)-H(37)	113(5)
Cu(3)-O(37)-H(37)	122(5)

Cu(2)-O(37)-H(37)	110(5)
C(6)-O(38)-Cu(1)	127.5(5)
C(6)-O(39)-Cu(4)	124.4(5)
C(3')-C(1)-C(2)	121(2)
C(3')-C(1)-H(1)	119.6
C(2)-C(1)-H(1)	119.6
C(1)-C(2)-C(3)	119.5(18)
C(1)-C(2)-C(6)	115.1(17)
C(3)-C(2)-C(6)	125.4(17)
C(4)-C(3)-C(2)	122(2)
C(4)-C(3)-C(1')	118.8(17)
C(2)-C(3)-C(1')	119.5(18)
C(5)-C(4)-C(3)	119.3(16)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(5')	122.6(15)
C(4)-C(5)-H(5)	118.7
C(5')-C(5)-H(5)	118.7
C(2')-C(1')-C(4')	122(2)
C(2')-C(1')-C(3)	118.8(17)
C(4')-C(1')-C(3)	119.5(19)
C(3')-C(2')-C(1')	121(2)
C(1)-C(3')-C(2')	120(2)
C(1)-C(3')-H(3')	119.8
C(2')-C(3')-H(3')	119.8
C(5')-C(4')-C(1')	120.3(18)
C(5')-C(4')-H(4')	119.9
C(1')-C(4')-H(4')	119.9
C(5)-C(5')-C(4')	119.1(16)
C(5)-C(5')-H(5')	120.4
C(4')-C(5')-H(5')	120.4
O(39)-C(6)-O(38)	126.5(7)
O(39)-C(6)-C(2)	118.7(11)
O(38)-C(6)-C(2)	114.1(11)
C(8)-N(1)-Cu(4)	107.3(6)
C(8)-N(1)-H(1A)	110.3
Cu(4)-N(1)-H(1A)	110.3
C(8)-N(1)-H(1B)	110.3

Cu(4)-N(1)-H(1B)	110.3
H(1A)-N(1)-H(1B)	108.5
C(9)-N(2)-Cu(4)	109.4(5)
C(9)-N(2)-H(2A)	109.8
Cu(4)-N(2)-H(2A)	109.8
C(9)-N(2)-H(2B)	109.8
Cu(4)-N(2)-H(2B)	109.8
H(2A)-N(2)-H(2B)	108.2
C(8)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-C(7)	120.3(12)
C(9)-C(8)-N(1)	106.7(9)
C(7)-C(8)-N(1)	112.4(11)
C(9)-C(8)-H(8)	105.4
C(7)-C(8)-H(8)	105.4
N(1)-C(8)-H(8)	105.4
N(2)-C(9)-C(8)	110.1(9)
N(2)-C(9)-H(9A)	109.6
C(8)-C(9)-H(9A)	109.6
N(2)-C(9)-H(9B)	109.6
C(8)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.2
C(11)-N(3)-Cu(5)	107.9(6)
C(11)-N(3)-H(3A)	110.1
Cu(5)-N(3)-H(3A)	110.1
C(11)-N(3)-H(3B)	110.1
Cu(5)-N(3)-H(3B)	110.1
H(3A)-N(3)-H(3B)	108.4
C(12)-N(4)-Cu(5)	108.0(6)
C(12)-N(4)-H(4A)	110.1
Cu(5)-N(4)-H(4A)	110.1
C(12)-N(4)-H(4B)	110.1
Cu(5)-N(4)-H(4B)	110.1
H(4A)-N(4)-H(4B)	108.4

C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12)	107.0(7)
N(3)-C(11)-C(10)	118.4(11)
C(12)-C(11)-C(10)	106.3(9)
N(3)-C(11)-H(11)	108.2
C(12)-C(11)-H(11)	108.2
C(10)-C(11)-H(11)	108.2
C(11)-C(12)-N(4)	107.6(7)
C(11)-C(12)-H(12A)	110.2
N(4)-C(12)-H(12A)	110.2
C(11)-C(12)-H(12B)	110.2
N(4)-C(12)-H(12B)	110.2
H(12A)-C(12)-H(12B)	108.5
C(11')-N(3')-Cu(5)	108.0(6)
C(11')-N(3')-H(3'A)	110.1
Cu(5)-N(3')-H(3'A)	110.1
C(11')-N(3')-H(3'B)	110.1
Cu(5)-N(3')-H(3'B)	110.1
H(3'A)-N(3')-H(3'B)	108.4
C(12')-N(4')-Cu(5)	107.9(6)
C(12')-N(4')-H(4'A)	110.1
Cu(5)-N(4')-H(4'A)	110.1
C(12')-N(4')-H(4'B)	110.1
Cu(5)-N(4')-H(4'B)	110.1
H(4'A)-N(4')-H(4'B)	108.4
C(11')-C(10')-H(10D)	109.5
C(11')-C(10')-H(10E)	109.5
H(10D)-C(10')-H(10E)	109.5
C(11')-C(10')-H(10F)	109.5
H(10D)-C(10')-H(10F)	109.5
H(10E)-C(10')-H(10F)	109.5
C(12')-C(11')-C(10')	95.8(13)
C(12')-C(11')-N(3')	107.6(7)

C(10')-C(11')-N(3')	126.8(14)
C(12')-C(11')-H(11')	108.3
C(10')-C(11')-H(11')	108.3
N(3')-C(11')-H(11')	108.3
N(4')-C(12')-C(11')	107.0(7)
N(4')-C(12')-H(12C)	110.3
C(11')-C(12')-H(12C)	110.3
N(4')-C(12')-H(12D)	110.3
C(11')-C(12')-H(12D)	110.3
H(12C)-C(12')-H(12D)	108.6
C(14)-N(5)-Cu(6)	108.8(6)
C(14)-N(5)-H(5A)	109.9
Cu(6)-N(5)-H(5A)	109.9
C(14)-N(5)-H(5B)	109.9
Cu(6)-N(5)-H(5B)	109.9
H(5A)-N(5)-H(5B)	108.3
C(15)-N(6)-Cu(6)	107.2(7)
C(15)-N(6)-H(6A)	110.3
Cu(6)-N(6)-H(6A)	110.3
C(15)-N(6)-H(6B)	110.3
Cu(6)-N(6)-H(6B)	110.3
H(6A)-N(6)-H(6B)	108.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(13)-C(14)-C(15)	118.2(17)
C(13)-C(14)-N(5)	124.4(15)
C(15)-C(14)-N(5)	107.5(9)
C(13)-C(14)-H(14)	100.5
C(15)-C(14)-H(14)	100.5
N(5)-C(14)-H(14)	100.5
N(6)-C(15)-C(14)	108.2(9)
N(6)-C(15)-H(15A)	110.1
C(14)-C(15)-H(15A)	110.1
N(6)-C(15)-H(15B)	110.1

C(14)-C(15)-H(15B)	110.1
H(15A)-C(15)-H(15B)	108.4
C(14')-N(5')-Cu(6)	107.2(7)
C(14')-N(5')-H(5'A)	110.3
Cu(6)-N(5')-H(5'A)	110.3
C(14')-N(5')-H(5'B)	110.3
Cu(6)-N(5')-H(5'B)	110.3
H(5'A)-N(5')-H(5'B)	108.5
C(15')-N(6')-Cu(6)	108.8(6)
C(15')-N(6')-H(6'A)	109.9
Cu(6)-N(6')-H(6'A)	109.9
C(15')-N(6')-H(6'B)	109.9
Cu(6)-N(6')-H(6'B)	109.9
H(6'A)-N(6')-H(6'B)	108.3
C(14')-C(13')-H(13D)	109.5
C(14')-C(13')-H(13E)	109.5
H(13D)-C(13')-H(13E)	109.5
C(14')-C(13')-H(13F)	109.5
H(13D)-C(13')-H(13F)	109.5
H(13E)-C(13')-H(13F)	109.5
N(5')-C(14')-C(13')	124.7(16)
N(5')-C(14')-C(15')	108.2(9)
C(13')-C(14')-C(15')	117.4(15)
N(5')-C(14')-H(14')	100.4
C(13')-C(14')-H(14')	100.4
C(15')-C(14')-H(14')	100.4
C(14')-C(15')-N(6')	107.5(9)
C(14')-C(15')-H(15C)	110.2
N(6')-C(15')-H(15C)	110.2
C(14')-C(15')-H(15D)	110.2
N(6')-C(15')-H(15D)	110.2
H(15C)-C(15')-H(15D)	108.5
C(17)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

N(7)-C(17)-C(18)	122(2)
N(7)-C(17)-C(16)	110(2)
C(18)-C(17)-C(16)	105.6(18)
N(7)-C(17)-H(17)	106.2
C(18)-C(17)-H(17)	106.2
C(16)-C(17)-H(17)	106.2
N(8)-C(18)-C(17)	101.8(18)
N(8)-C(18)-H(18A)	111.4
C(17)-C(18)-H(18A)	111.4
N(8)-C(18)-H(18B)	111.4
C(17)-C(18)-H(18B)	111.4
H(18A)-C(18)-H(18B)	109.3
C(17)-N(7)-Cu(7)	105.0(15)
C(17)-N(7)-H(7D)	110.7
Cu(7)-N(7)-H(7D)	110.7
C(17)-N(7)-H(7E)	110.7
Cu(7)-N(7)-H(7E)	110.7
H(7D)-N(7)-H(7E)	108.8
C(18)-N(8)-Cu(7)	112.0(15)
C(18)-N(8)-H(8A)	109.2
Cu(7)-N(8)-H(8A)	109.2
C(18)-N(8)-H(8B)	109.2
Cu(7)-N(8)-H(8B)	109.2
H(8A)-N(8)-H(8B)	107.9
N(7)-Cu(7)-N(8)	87.5(9)
N(7)-Cu(7)-O(19)	102.3(9)
N(8)-Cu(7)-O(19)	97.6(5)
N(7)-Cu(7)-Cl(1A)	164.5(9)
N(8)-Cu(7)-Cl(1A)	93.1(6)
O(19)-Cu(7)-Cl(1A)	93.1(2)
N(7)-Cu(7)-O(43)	77.8(11)
N(8)-Cu(7)-O(43)	164.8(11)
O(19)-Cu(7)-O(43)	89.2(9)
Cl(1A)-Cu(7)-O(43)	100.1(9)
O(42)-Cu(7')-O(19)	90.5(7)
O(42)-Cu(7')-O(43A)	128.3(9)
O(19)-Cu(7')-O(43A)	71.9(5)
Cl(1)-Na(1)-O(19)	85.9(6)

Cl(1)-Na(1)-O(47)	101.3(9)
O(19)-Na(1)-O(47)	61.9(5)
Cl(1)-Na(1)-O(43B)	97.5(11)
O(19)-Na(1)-O(43B)	102.4(7)
O(47)-Na(1)-O(43B)	154.3(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+3/2 #2 -x+1,y+1/2,-z+3/2

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for platon_sq. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	7(1)	7(1)	14(1)	2(1)	-2(1)	1(1)
W(1)	11(1)	11(1)	34(1)	-2(1)	-1(1)	4(1)
W(2)	25(1)	10(1)	21(1)	5(1)	-7(1)	1(1)
W(3)	18(1)	17(1)	32(1)	0(1)	-15(1)	4(1)
W(4)	13(1)	11(1)	17(1)	-1(1)	3(1)	1(1)
W(5)	13(1)	9(1)	18(1)	1(1)	1(1)	-3(1)
W(6)	28(1)	14(1)	13(1)	3(1)	3(1)	-2(1)
W(7)	23(1)	18(1)	16(1)	-3(1)	-10(1)	3(1)
W(8)	10(1)	12(1)	38(1)	-2(1)	-7(1)	-1(1)
W(9)	11(1)	10(1)	33(1)	1(1)	10(1)	0(1)
Cu(1)	12(1)	12(1)	12(1)	2(1)	2(1)	2(1)
Cu(2)	10(1)	14(1)	15(1)	1(1)	0(1)	0(1)
Cu(3)	10(1)	12(1)	13(1)	-1(1)	1(1)	-1(1)
Cu(4)	12(1)	21(1)	19(1)	-4(1)	-2(1)	2(1)
Cu(5)	19(1)	10(1)	25(1)	2(1)	9(1)	0(1)
Cu(6)	17(1)	23(1)	18(1)	-3(1)	2(1)	-1(1)
O(1)	18(2)	11(2)	30(3)	2(2)	-3(2)	4(2)
O(2)	25(2)	18(2)	27(3)	2(2)	-11(2)	0(2)
O(3)	17(2)	14(2)	36(3)	-4(2)	-7(2)	4(2)
O(4)	18(2)	20(2)	58(4)	-9(2)	0(2)	8(2)
O(5)	48(3)	16(2)	36(3)	12(2)	-12(3)	-1(2)
O(6)	29(3)	31(3)	49(4)	-1(3)	-24(3)	9(2)
O(7)	15(2)	12(2)	30(3)	-2(2)	4(2)	1(2)
O(8)	22(2)	11(2)	22(2)	6(2)	-1(2)	-1(2)
O(9)	39(3)	14(2)	18(2)	6(2)	-4(2)	-2(2)
O(10)	30(3)	21(2)	25(3)	-1(2)	-17(2)	-1(2)
O(11)	10(2)	19(2)	42(3)	-3(2)	-13(2)	2(2)
O(12)	8(2)	16(2)	41(3)	-2(2)	5(2)	4(2)
O(13)	15(2)	10(2)	19(2)	-2(2)	1(2)	-1(2)

O(14)	22(2)	15(2)	19(2)	2(2)	5(2)	-7(2)
O(15)	30(3)	20(2)	14(2)	1(2)	-3(2)	-2(2)
O(16)	17(2)	15(2)	33(3)	-2(2)	-13(2)	-2(2)
O(17)	11(2)	13(2)	34(3)	-2(2)	0(2)	-3(2)
O(18)	16(2)	14(2)	28(3)	0(2)	11(2)	-1(2)
O(19)	31(3)	22(2)	22(3)	-7(2)	4(2)	0(2)
O(20)	17(2)	11(2)	31(3)	-1(2)	0(2)	-5(2)
O(21)	44(3)	27(3)	19(3)	6(2)	8(2)	-5(2)
O(22)	42(3)	32(3)	19(3)	-9(2)	-7(2)	2(2)
O(23)	20(3)	18(2)	65(4)	-4(2)	-9(3)	-5(2)
O(24)	25(3)	18(2)	56(4)	1(2)	26(3)	0(2)
O(25)	16(2)	16(2)	18(2)	0(2)	2(2)	0(2)
O(26)	13(2)	11(2)	17(2)	-2(2)	0(2)	1(2)
O(27)	19(2)	13(2)	19(2)	-1(2)	1(2)	-3(2)
O(28)	13(2)	15(2)	16(2)	0(2)	-3(2)	-1(2)
O(29)	14(2)	10(2)	25(2)	1(2)	0(2)	-1(2)
O(30)	15(2)	11(2)	20(2)	3(2)	9(2)	2(2)
O(31)	9(2)	8(2)	21(2)	1(2)	1(2)	2(1)
O(32)	12(2)	11(2)	17(2)	3(2)	-3(2)	-2(2)
O(33)	11(2)	12(2)	24(2)	0(2)	-6(2)	-1(2)
O(34)	11(2)	9(2)	15(2)	1(2)	1(2)	3(2)
O(35)	13(2)	14(2)	16(2)	-1(2)	-2(2)	5(2)
O(36)	14(2)	12(2)	19(2)	2(2)	2(2)	5(2)
O(37)	10(2)	14(2)	19(2)	0(2)	-1(2)	4(2)
O(38)	35(3)	22(2)	20(3)	4(2)	-2(2)	0(2)
O(39)	51(4)	56(4)	23(3)	12(3)	-16(3)	-20(3)
O(40)	85(5)	19(3)	35(3)	3(2)	5(3)	15(3)
O(41)	16(3)	44(3)	62(4)	-14(3)	1(3)	-3(2)
C(1)	37(8)	43(8)	18(5)	3(5)	0(6)	5(6)
C(2)	28(5)	28(5)	23(3)	8(3)	-5(4)	5(4)
C(3)	46(8)	42(8)	18(4)	12(5)	-5(7)	3(7)
C(4)	28(8)	38(8)	23(8)	4(6)	1(6)	4(6)
C(5)	41(9)	46(10)	29(9)	13(7)	3(7)	16(8)
C(1')	37(8)	43(8)	18(5)	3(5)	0(6)	5(6)
C(2')	28(5)	28(5)	23(3)	8(3)	-5(4)	5(4)
C(3')	46(8)	42(8)	18(4)	12(5)	-5(7)	3(7)
C(4')	40(10)	62(12)	24(8)	16(8)	14(7)	10(9)
C(5')	42(11)	94(17)	32(10)	18(10)	10(8)	13(11)

C(6)	40(4)	34(4)	18(4)	6(3)	-3(3)	1(3)
N(1)	23(3)	37(4)	46(4)	-21(3)	-11(3)	-2(3)
N(2)	14(3)	52(4)	29(3)	-11(3)	0(2)	0(3)
C(7)	98(12)	97(12)	200(20)	-71(13)	-36(13)	-31(10)
C(8)	43(6)	50(6)	144(13)	-32(7)	-23(7)	-2(5)
C(9)	23(4)	104(10)	92(9)	-68(8)	-1(5)	-6(5)
N(3)	66(5)	11(3)	26(3)	4(2)	22(3)	6(3)
N(4)	30(3)	15(3)	64(5)	3(3)	23(3)	-7(2)
C(10)	47(8)	47(8)	36(7)	7(6)	19(6)	1(6)
C(11)	108(9)	22(4)	50(6)	-2(4)	55(6)	-2(5)
C(12)	84(8)	22(4)	71(7)	-4(4)	56(6)	-16(4)
N(3')	30(3)	15(3)	64(5)	3(3)	23(3)	-7(2)
N(4')	66(5)	11(3)	26(3)	4(2)	22(3)	6(3)
C(10')	30(13)	42(14)	53(17)	6(12)	6(12)	-9(11)
C(11')	84(8)	22(4)	71(7)	-4(4)	56(6)	-16(4)
C(12')	108(9)	22(4)	50(6)	-2(4)	55(6)	-2(5)
N(5)	21(3)	76(6)	39(4)	-12(4)	6(3)	-2(3)
N(6)	54(5)	41(4)	21(3)	0(3)	6(3)	8(3)
C(13)	50(13)	170(30)	62(15)	-54(17)	17(11)	-22(16)
C(14)	45(6)	130(12)	66(8)	-3(8)	33(6)	13(7)
C(15)	70(8)	83(9)	81(9)	39(7)	57(7)	20(7)
N(5')	54(5)	41(4)	21(3)	0(3)	6(3)	8(3)
N(6')	21(3)	76(6)	39(4)	-12(4)	6(3)	-2(3)
C(13')	120(20)	87(19)	44(14)	4(13)	29(14)	-27(17)
C(14')	70(8)	83(9)	81(9)	39(7)	57(7)	20(7)
C(15')	45(6)	130(12)	66(8)	-3(8)	33(6)	13(7)
C(16)	180(20)	160(20)	160(20)	40(20)	0(20)	-40(20)
C(17)	122(11)	122(11)	79(9)	30(9)	20(9)	-29(9)
C(18)	107(12)	124(12)	60(10)	29(9)	15(10)	-36(10)
N(7)	127(12)	121(11)	89(10)	31(9)	27(10)	-22(10)
N(8)	82(9)	62(8)	39(7)	-24(7)	-7(7)	-1(7)
Cl(1A)	17(3)	18(3)	10(3)	-6(2)	2(2)	-5(2)
O(42A)	17(3)	18(3)	10(3)	-6(2)	2(2)	-5(2)
Cu(7)	46(1)	41(1)	26(1)	-4(1)	5(1)	-4(1)
O(43)	89(15)	89(14)	84(15)	-8(9)	-4(9)	-3(9)
Cu(7')	39(4)	38(4)	30(4)	-3(3)	6(3)	-7(3)
O(42)	42(9)	11(7)	51(10)	-8(7)	18(8)	6(7)
O(43A)	81(15)	79(14)	37(10)	-2(10)	-26(10)	-9(12)

Cl(1)	41(5)	37(5)	24(4)	-7(3)	-3(3)	-7(3)
Na(1)	35(6)	42(6)	33(6)	-16(5)	4(5)	14(6)
O(43B)	80(20)	140(30)	29(14)	-36(16)	6(15)	-20(20)
O(47)	85(10)	74(9)	46(8)	-34(8)	-27(8)	32(8)
O(44)	39(4)	33(3)	93(6)	-22(3)	-2(4)	-10(3)
O(45)	70(5)	32(3)	96(6)	27(4)	-20(4)	8(3)
O(46)	84(6)	55(5)	110(7)	-26(5)	38(5)	12(4)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon_sq.

x	y	z	U(eq)
H(35)	6920(50)	5570(20)	7970(30)	17
H(36)	5120(50)	4350(20)	7710(30)	18
H(37)	6760(50)	4930(20)	7030(30)	17
H(1)	6879	5132	9763	39
H(4)	3061	5691	9082	36
H(5)	1088	5626	9359	46
H(3')	6453	4691	10531	43
H(4')	2240	4812	10640	50
H(5')	680	5296	10156	67
H(1A)	6142	7820	8504	43
H(1B)	6436	7507	8982	43
H(2A)	8532	6236	8561	38
H(2B)	8638	6644	8117	38
H(7A)	8015	8328	9236	197
H(7B)	7718	8726	8741	197
H(7C)	9079	8488	8865	197
H(8)	8072	7845	8266	95
H(9A)	9576	7267	8655	88
H(9B)	8666	7049	9076	88
H(3A)	3635	3749	8480	41
H(3B)	3749	4439	8631	41
H(4A)	802	4551	7899	43
H(4B)	972	3942	7618	43
H(10A)	1184	3817	9310	65
H(10B)	2627	3861	9395	65
H(10C)	2044	3263	9093	65
H(11)	1782	4563	8763	71
H(12A)	388	3800	8468	70
H(12B)	1468	3342	8282	70
H(3'A)	802	4551	7899	43
H(3'B)	972	3942	7618	43
H(4'A)	3635	3749	8480	41

H(4'B)	3749	4439	8631	41
H(10D)	348	3413	8926	63
H(10E)	-562	3643	8491	63
H(10F)	71	4173	8846	63
H(11')	1521	3348	8274	70
H(12C)	1782	4551	8786	71
H(12D)	2130	3844	9006	71
H(5A)	8488	5547	6325	54
H(5B)	8271	4837	6301	54
H(6A)	6029	5218	5336	46
H(6B)	5817	5917	5439	46
H(13A)	9523	5015	5098	143
H(13B)	9988	4779	5631	143
H(13C)	10054	5535	5487	143
H(14)	7956	4816	5524	96
H(15A)	7788	6160	5502	92
H(15B)	7664	5694	5028	92
H(5'A)	6029	5218	5336	46
H(5'B)	5817	5917	5439	46
H(6'A)	8488	5547	6325	54
H(6'B)	8271	4837	6301	54
H(13D)	7760	5650	4654	123
H(13E)	8831	6051	4927	123
H(13F)	7522	6379	4840	123
H(14')	7726	6104	5603	92
H(15C)	9225	5348	5594	96
H(15D)	8218	4793	5490	96
H(16A)	1343	6487	9752	252
H(16B)	380	6869	10076	252
H(16C)	1439	6451	10339	252
H(17)	2110	7477	10416	129
H(18A)	995	7687	9472	116
H(18B)	690	8039	9986	116
H(7D)	3248	6811	9719	134
H(7E)	3711	7031	10207	134
H(8A)	2321	8629	9955	74
H(8B)	2104	8565	9421	74

Table S7. Torsion angles [°] for platon_sq.

O(6)-W(3)-O(2)-W(2)	133.2(6)
O(11)-W(3)-O(2)-W(2)	-42.8(10)
O(10)-W(3)-O(2)-W(2)	-125.6(6)
O(3)-W(3)-O(2)-W(2)	31.7(6)
O(33)-W(3)-O(2)-W(2)	-53.3(6)
O(4)-W(1)-O(7)-W(4)	165.6(3)
O(12)-W(1)-O(7)-W(4)	63.9(3)
O(1)-W(1)-O(7)-W(4)	-91.6(3)
O(3)-W(1)-O(7)-W(4)	-21.9(7)
O(31)-W(1)-O(7)-W(4)	-6.9(2)
O(5)-W(2)-O(8)-W(5)	-168.0(3)
O(9)-W(2)-O(8)-W(5)	-65.4(3)
O(1)-W(2)-O(8)-W(5)	89.7(3)
O(2)-W(2)-O(8)-W(5)	19.9(7)
O(32)-W(2)-O(8)-W(5)	5.6(2)
O(5)-W(2)-O(9)-W(6)	166.7(3)
O(8)-W(2)-O(9)-W(6)	63.7(3)
O(1)-W(2)-O(9)-W(6)	-27.1(7)
O(2)-W(2)-O(9)-W(6)	-91.6(3)
O(32)-W(2)-O(9)-W(6)	-7.6(2)
O(4)-W(1)-O(12)-W(9)	-168.2(3)
O(7)-W(1)-O(12)-W(9)	-67.9(3)
O(1)-W(1)-O(12)-W(9)	16.8(7)
O(3)-W(1)-O(12)-W(9)	89.6(3)
O(31)-W(1)-O(12)-W(9)	4.2(3)
O(19)-W(4)-O(18)-W(9)	178.0(3)
O(25)-W(4)-O(18)-W(9)	-77.3(3)
O(13)-W(4)-O(18)-W(9)	16.0(6)
O(7)-W(4)-O(18)-W(9)	80.6(3)
O(31)-W(4)-O(18)-W(9)	8.1(2)
O(25)-W(4)-O(19)-Cu(7)	-71.5(10)
O(18)-W(4)-O(19)-Cu(7)	24.7(10)
O(13)-W(4)-O(19)-Cu(7)	-162.3(9)
O(7)-W(4)-O(19)-Cu(7)	110.9(9)
O(31)-W(4)-O(19)-Cu(7)	87.7(14)
O(25)-W(4)-O(19)-Cu(7')	-167.1(14)

O(18)-W(4)-O(19)-Cu(7')	-70.9(14)
O(13)-W(4)-O(19)-Cu(7')	102.1(14)
O(7)-W(4)-O(19)-Cu(7')	15.3(14)
O(31)-W(4)-O(19)-Cu(7')	-8(2)
O(25)-W(4)-O(19)-Na(1)	-34.1(10)
O(18)-W(4)-O(19)-Na(1)	62.2(9)
O(13)-W(4)-O(19)-Na(1)	-124.9(9)
O(7)-W(4)-O(19)-Na(1)	148.4(9)
O(31)-W(4)-O(19)-Na(1)	125.1(11)
O(26)-W(5)-O(20)-Cu(5)#2	147.6(3)
O(13)-W(5)-O(20)-Cu(5)#2	-113.4(3)
O(14)-W(5)-O(20)-Cu(5)#2	54.4(3)
O(8)-W(5)-O(20)-Cu(5)#2	-27.8(3)
O(19)-W(4)-O(25)-Cu(4)	-54.6(4)
O(18)-W(4)-O(25)-Cu(4)	-157.1(4)
O(13)-W(4)-O(25)-Cu(4)	45.9(4)
O(7)-W(4)-O(25)-Cu(4)	119.0(5)
O(31)-W(4)-O(25)-Cu(4)	129.2(4)
O(19)-W(4)-O(25)-Cu(1)	145.0(3)
O(18)-W(4)-O(25)-Cu(1)	42.6(3)
O(13)-W(4)-O(25)-Cu(1)	-114.5(3)
O(7)-W(4)-O(25)-Cu(1)	-41.4(7)
O(31)-W(4)-O(25)-Cu(1)	-31.1(3)
O(20)-W(5)-O(26)-Cu(3)	-146.1(3)
O(13)-W(5)-O(26)-Cu(3)	112.0(4)
O(14)-W(5)-O(26)-Cu(3)	-45.8(4)
O(8)-W(5)-O(26)-Cu(3)	22.4(7)
O(32)-W(5)-O(26)-Cu(3)	28.3(3)
O(21)-W(6)-O(27)-Cu(3)	150.4(4)
O(14)-W(6)-O(27)-Cu(3)	47.0(4)
O(15)-W(6)-O(27)-Cu(3)	-108.7(4)
O(9)-W(6)-O(27)-Cu(3)	-24.3(7)
O(32)-W(6)-O(27)-Cu(3)	-26.2(3)
O(21)-W(6)-O(27)-Cu(6)	-67.2(3)
O(14)-W(6)-O(27)-Cu(6)	-170.6(3)
O(15)-W(6)-O(27)-Cu(6)	33.7(3)
O(9)-W(6)-O(27)-Cu(6)	118.1(4)
O(32)-W(6)-O(27)-Cu(6)	116.2(2)

O(22)-W(7)-O(28)-Cu(2)	-141.5(3)
O(15)-W(7)-O(28)-Cu(2)	117.5(3)
O(16)-W(7)-O(28)-Cu(2)	-38.5(3)
O(10)-W(7)-O(28)-Cu(2)	34.3(7)
O(33)-W(7)-O(28)-Cu(2)	34.9(3)
O(22)-W(7)-O(28)-Cu(6)	59.6(3)
O(15)-W(7)-O(28)-Cu(6)	-41.3(3)
O(16)-W(7)-O(28)-Cu(6)	162.7(3)
O(10)-W(7)-O(28)-Cu(6)	-124.5(5)
O(33)-W(7)-O(28)-Cu(6)	-124.0(3)
O(23)-W(8)-O(29)-Cu(2)	142.8(3)
O(16)-W(8)-O(29)-Cu(2)	40.1(3)
O(17)-W(8)-O(29)-Cu(2)	-116.2(3)
O(11)-W(8)-O(29)-Cu(2)	-31.7(7)
O(33)-W(8)-O(29)-Cu(2)	-33.9(3)
O(23)-W(8)-O(29)-Cu(5)	-58.6(3)
O(16)-W(8)-O(29)-Cu(5)	-161.2(3)
O(17)-W(8)-O(29)-Cu(5)	42.4(3)
O(11)-W(8)-O(29)-Cu(5)	126.9(5)
O(33)-W(8)-O(29)-Cu(5)	124.7(3)
O(24)-W(9)-O(30)-Cu(1)	-150.1(4)
O(17)-W(9)-O(30)-Cu(1)	109.4(4)
O(18)-W(9)-O(30)-Cu(1)	-48.3(4)
O(12)-W(9)-O(30)-Cu(1)	22.8(8)
O(31)-W(9)-O(30)-Cu(1)	25.2(4)
O(24)-W(9)-O(30)-Cu(5)	65.9(3)
O(17)-W(9)-O(30)-Cu(5)	-34.7(3)
O(18)-W(9)-O(30)-Cu(5)	167.6(2)
O(12)-W(9)-O(30)-Cu(5)	-121.3(4)
O(31)-W(9)-O(30)-Cu(5)	-118.9(2)
O(34)-P(1)-O(31)-W(9)	-56.3(3)
O(33)-P(1)-O(31)-W(9)	64.3(3)
O(32)-P(1)-O(31)-W(9)	-178.1(2)
O(34)-P(1)-O(31)-W(4)	58.5(3)
O(33)-P(1)-O(31)-W(4)	179.1(2)
O(32)-P(1)-O(31)-W(4)	-63.3(3)
O(34)-P(1)-O(31)-W(1)	-177.9(2)
O(33)-P(1)-O(31)-W(1)	-57.3(3)

O(32)-P(1)-O(31)-W(1)	60.3(3)
O(34)-P(1)-O(32)-W(5)	-57.3(3)
O(33)-P(1)-O(32)-W(5)	-179.0(2)
O(31)-P(1)-O(32)-W(5)	63.2(3)
O(34)-P(1)-O(32)-W(6)	61.0(3)
O(33)-P(1)-O(32)-W(6)	-60.8(3)
O(31)-P(1)-O(32)-W(6)	-178.5(2)
O(34)-P(1)-O(32)-W(2)	-178.3(2)
O(33)-P(1)-O(32)-W(2)	59.9(3)
O(31)-P(1)-O(32)-W(2)	-57.9(3)
O(34)-P(1)-O(33)-W(8)	56.5(3)
O(31)-P(1)-O(33)-W(8)	-63.7(3)
O(32)-P(1)-O(33)-W(8)	179.1(2)
O(34)-P(1)-O(33)-W(7)	-62.3(3)
O(31)-P(1)-O(33)-W(7)	177.5(2)
O(32)-P(1)-O(33)-W(7)	60.4(3)
O(34)-P(1)-O(33)-W(3)	177.7(3)
O(31)-P(1)-O(33)-W(3)	57.5(3)
O(32)-P(1)-O(33)-W(3)	-59.6(3)
O(33)-P(1)-O(34)-Cu(1)	-118.9(3)
O(31)-P(1)-O(34)-Cu(1)	0.8(4)
O(32)-P(1)-O(34)-Cu(1)	120.3(3)
O(33)-P(1)-O(34)-Cu(3)	116.5(3)
O(31)-P(1)-O(34)-Cu(3)	-123.8(3)
O(32)-P(1)-O(34)-Cu(3)	-4.3(3)
O(33)-P(1)-O(34)-Cu(2)	5.7(3)
O(31)-P(1)-O(34)-Cu(2)	125.3(3)
O(32)-P(1)-O(34)-Cu(2)	-115.2(3)
C(3')-C(1)-C(2)-C(3)	3(4)
C(3')-C(1)-C(2)-C(6)	-176(3)
C(1)-C(2)-C(3)-C(4)	175(3)
C(6)-C(2)-C(3)-C(4)	-6(5)
C(1)-C(2)-C(3)-C(1')	0(4)
C(6)-C(2)-C(3)-C(1')	179(2)
C(2)-C(3)-C(4)-C(5)	-178(3)
C(1')-C(3)-C(4)-C(5)	-3(4)
C(3)-C(4)-C(5)-C(5')	4(3)
C(4)-C(3)-C(1')-C(2')	-179(3)

C(2)-C(3)-C(1')-C(2')	-4(4)
C(4)-C(3)-C(1')-C(4')	3(4)
C(2)-C(3)-C(1')-C(4')	179(3)
C(4')-C(1')-C(2')-C(3')	-178(3)
C(3)-C(1')-C(2')-C(3')	5(4)
C(2)-C(1)-C(3')-C(2')	-1(5)
C(1')-C(2')-C(3')-C(1)	-2(4)
C(2')-C(1')-C(4')-C(5')	177(2)
C(3)-C(1')-C(4')-C(5')	-5(4)
C(4)-C(5)-C(5')-C(4')	-6(3)
C(1')-C(4')-C(5')-C(5)	7(3)
Cu(4)-O(39)-C(6)-O(38)	13.1(13)
Cu(4)-O(39)-C(6)-C(2)	-157.3(9)
Cu(1)-O(38)-C(6)-O(39)	-15.8(12)
Cu(1)-O(38)-C(6)-C(2)	154.9(9)
C(1)-C(2)-C(6)-O(39)	-57(2)
C(3)-C(2)-C(6)-O(39)	124(3)
C(1)-C(2)-C(6)-O(38)	131(2)
C(3)-C(2)-C(6)-O(38)	-48(3)
Cu(4)-N(1)-C(8)-C(9)	-40.8(12)
Cu(4)-N(1)-C(8)-C(7)	-174.7(12)
Cu(4)-N(2)-C(9)-C(8)	-36.3(13)
C(7)-C(8)-C(9)-N(2)	-179.6(14)
N(1)-C(8)-C(9)-N(2)	50.9(14)
Cu(5)-N(3)-C(11)-C(12)	42.2(8)
Cu(5)-N(3)-C(11)-C(10)	162.1(9)
N(3)-C(11)-C(12)-N(4)	-54.6(9)
C(10)-C(11)-C(12)-N(4)	178.0(8)
Cu(5)-N(4)-C(12)-C(11)	40.4(8)
Cu(5)-N(3')-C(11')-C(12')	40.4(8)
Cu(5)-N(3')-C(11')-C(10')	152.1(15)
Cu(5)-N(4')-C(12')-C(11')	42.2(8)
C(10')-C(11')-C(12')-N(4')	173.8(12)
N(3')-C(11')-C(12')-N(4')	-54.6(9)
Cu(6)-N(5)-C(14)-C(13)	-180(2)
Cu(6)-N(5)-C(14)-C(15)	35.4(13)
Cu(6)-N(6)-C(15)-C(14)	44.2(12)
C(13)-C(14)-C(15)-N(6)	159.9(16)

N(5)-C(14)-C(15)-N(6)	-52.7(15)
Cu(6)-N(5')-C(14')-C(13')	-171.1(16)
Cu(6)-N(5')-C(14')-C(15')	44.2(12)
N(5')-C(14')-C(15')-N(6')	-52.7(15)
C(13')-C(14')-C(15')-N(6')	159.6(16)
Cu(6)-N(6')-C(15')-C(14')	35.4(13)
N(7)-C(17)-C(18)-N(8)	-40(3)
C(16)-C(17)-C(18)-N(8)	-166(3)
C(18)-C(17)-N(7)-Cu(7)	27(3)
C(16)-C(17)-N(7)-Cu(7)	152(2)
C(17)-C(18)-N(8)-Cu(7)	31(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+3/2 #2 -x+1,y+1/2,-z+3/2

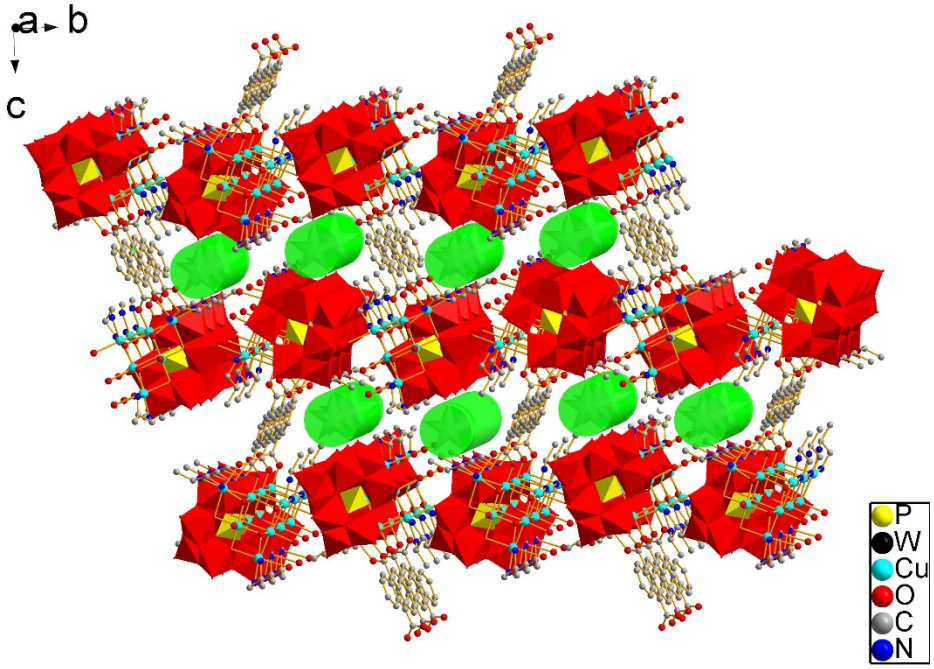

Fig. S1. View of stacking fashion of Cu-POMCOF in *bc* plane, the counter cations are omitted for clarify.

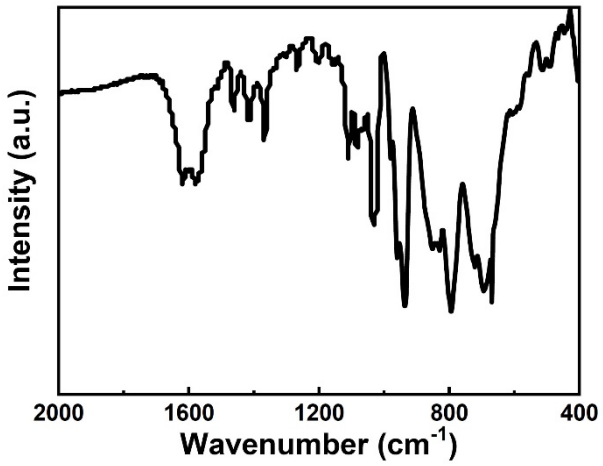

Fig. S2. IR spectra of Cu-POMCOF: 3436 (m), 3323 (m), 3256 (m), 2967(w), 2879(w), 2357 (w), 2338 (w), 1620 (m), 1563 (m), 1465 (w), 1369 (m), 1269 (w), 1105 (w), 1030 (s), 959 (m), 945 (s), 854 (m), 795 (s), 720 (m),691 (s), 670 (s).

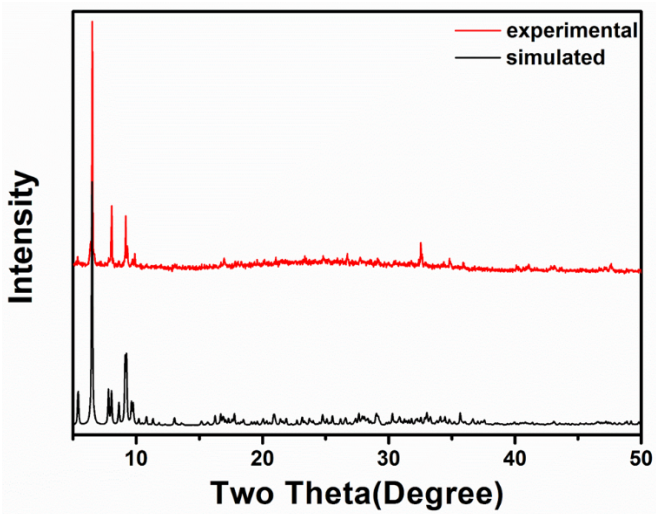

Fig. S3. The simulated and experimental PXRD patterns of Cu-POMCOF.

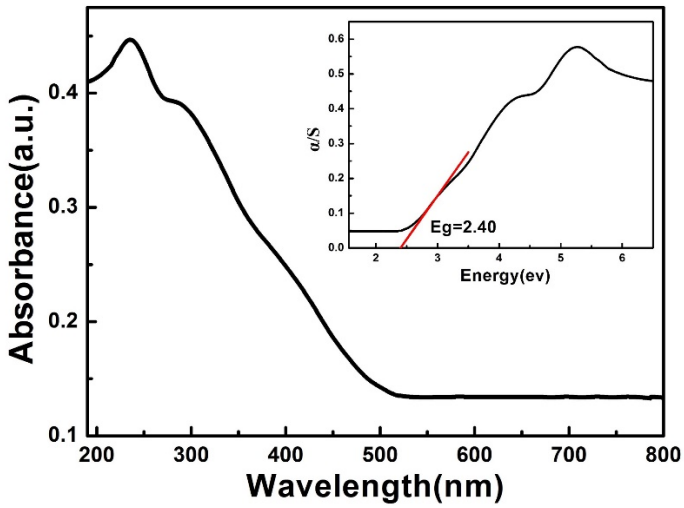

Fig. S4. UV/Vis-NIR diffuse reflectance spectrum of Cu-POMCOF.

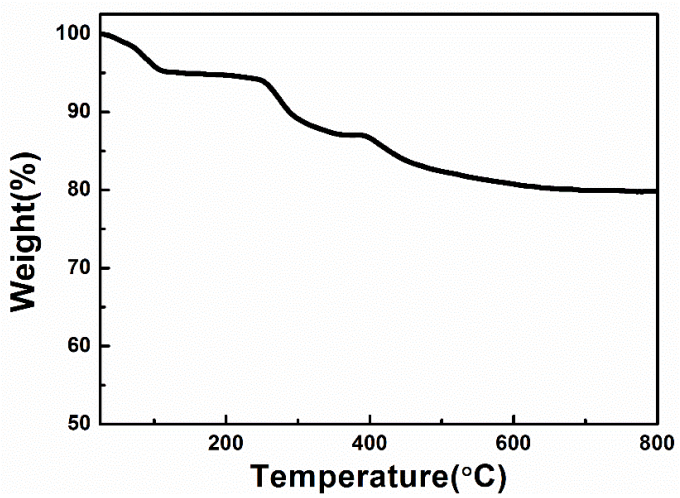

Fig. S5. The TG curves of Cu-POMCOF.

The thermogravimatric behaviors of **1** were investigated in the flowing air atmosphere from 25 to 1000 °C.

For Cu-POMCOF, the first weight loss of 5.18% from 25 to 170 °C is assigned to release of 2 lattice water molecules and [Na(dap)(H_2O)$_2$] (calcd. 4.99%). From 170 to 370 °C, the weight loss of 8.29% corresponds to release of 4 coordination water molecules and 3 dap groups (calcd. 8.13%).

Enzyme encapsulation

Introducing 0.5 mg Cu-POMCOF to MP-11 solution (1 mg/mL) and Cyt C(1 mg/ml) solution separately, then incubating with gently shaken for 3 h at room temperature (25±2 ℃). After that, mixture were centrifuged at 12000 g for 10 min and supernatant containing unloaded enzyme was carefully removed. The concentration of unloaded enzyme presented in supernatant was determined by UV-vis with an absorbance of 399 nm at different time. Then the concentration of loaded enzyme could be calculated by subtracting the amount of unloaded enzyme from initial enzyme solution. The precipitation contained immobilized enzyme was then washed 3 times with deionized water to remove unloaded enzyme and stored at 0 ℃ for further using.

Measurement of enzyme activity

To measure the activity of immobilized enzyme and free enzyme, 5 mM MP-11 and MP-11@Cu-POMCOF contain equivalent amount of immobilized MP-11 was mixed with 2 mM ABTS, 10 mM H_2O_2 in 300 μL of 0.1 M citric acid-sodium citrate buffer(pH=6). Then enzyme activities were obtained spectrophotometrically at 418 nm in a UV 3600 spectrophotometer (Shimadzu, Japan) at different time

When study enzyme specific activities in different buffer, citric acid-sodium citrate buffer was replaced by deionized water or organic buffer =1:1 with same ingredient and condition. The activity of Cyt c and Cyt c@Cu-POMCOF were using same method as described above.

Kinetic analysis

In order to study the enzymatic kinetics parameters, the catalytic activity of different

group was measured with different of ABTS substrate concentrations ranging from 0.1-2.2 mM. Results were then fitting with Michaelis-Menten equation.

$$V=V_{max}\,S/(K_m+S)$$

In this equation, V stands for reaction velocity($mmol^{-1}$ min^{-1}), S is the substrate concentration, and K_m is the Michealis-Menten constant, stands for the affinity between the enzyme and the substrate. K_m and V_{max} could be obtained by fitting with nonlinear regression equation.

Enzyme recycling and leaking study

For enzyme recycling, the reaction was conducted with same condition describe above. After the reaction was completed, the precipitation was collected by centrifugation at 1,2000g, the supernatant was collected for leaking experiment. Wash the pellet twice with deionized water and then used for next reaction, repeated for a total of five times. The enzyme activity testing method was the same as described previously. Meanwhile, by measuring enzyme concentration in supernatant after each cycle, we can learn how much enzyme was leaking from Cu-POMCOF.

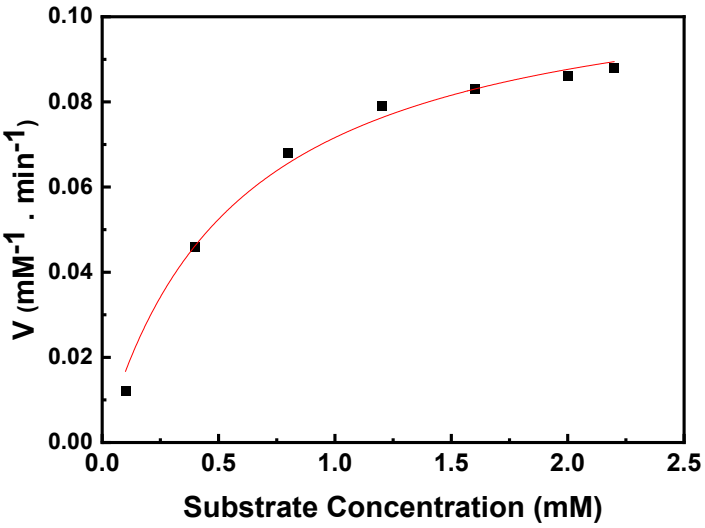

Fig. S6. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free MP-11 in acid-sodium citrate buffer. The reactions were performed with 2 mM ABTS, 0.1-2.2 mM H_2O_2, 5 mM enzyme room temperature.

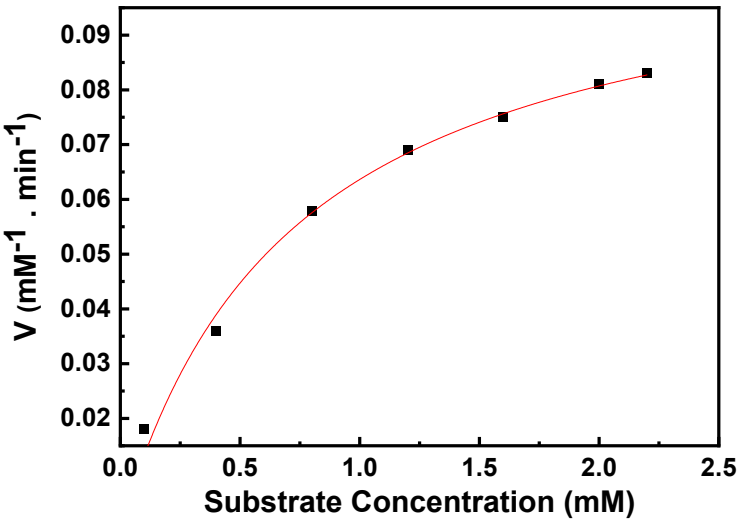

Fig. S7. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free MP-11@Cu-POMCOF in acid-sodium citrate buffer. The reactions were performed with 2 mM ABTS, 0.1-2.2 mM H_2O_2, 5 mM enzyme room temperature.

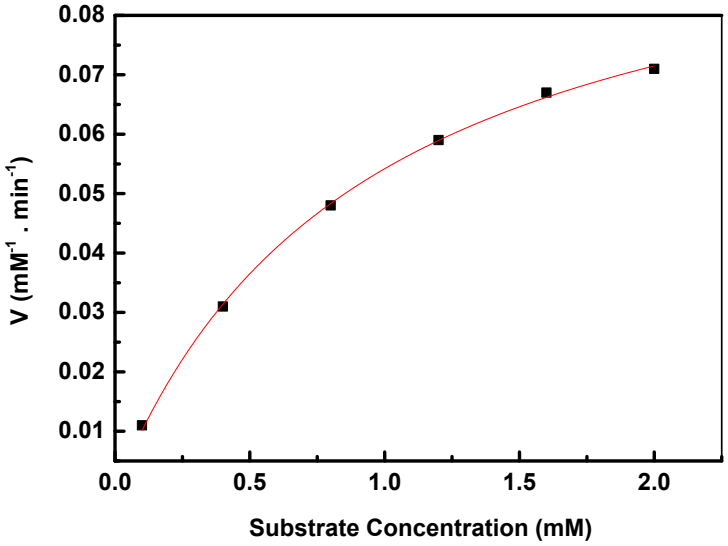

Fig. S8. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free Cyt C in acid-sodium citrate buffer. The reactions were performed with 2 mM ABTS, 0.1-2.2 mM H_2O_2, 5 mM enzyme room temperature.

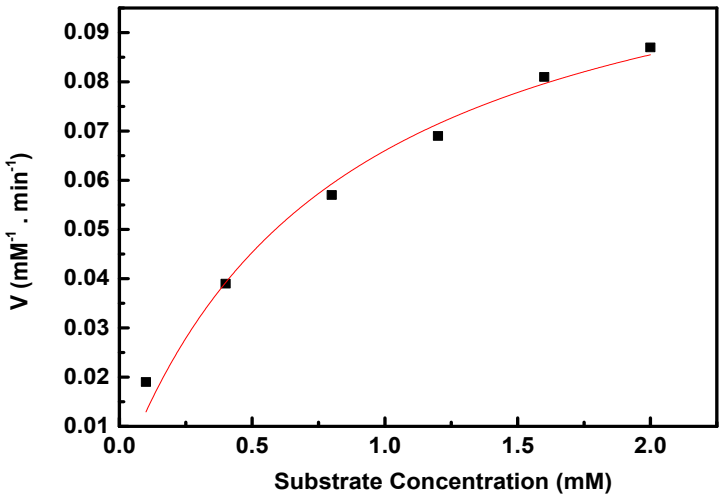

Fig. S9. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free Cyt C@Cu-PMOF in acid-sodium citrate buffer. The reactions were performed with 2 mM ABTS, 0.1-2.0 mM H_2O_2, 5 mM enzyme room temperature.

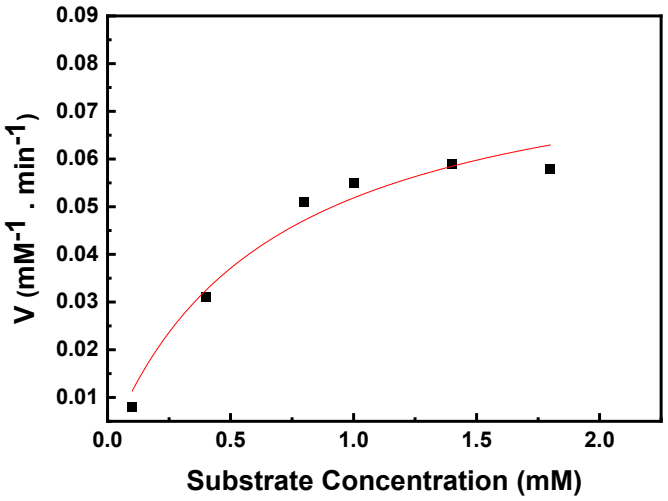

Fig. S10. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free Cyt C in water. The reactions were performed with 2 mM ABTS, 0.1-2.2 mM H_2O_2, 5 mM enzyme room temperature.

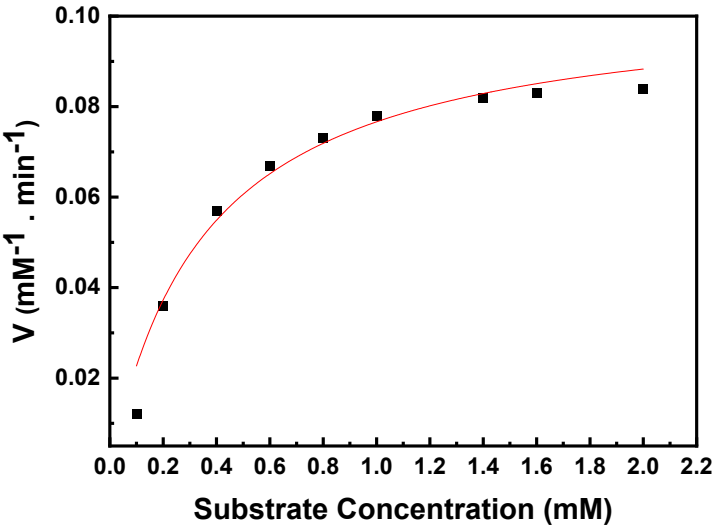

Fig. S11. The Michaelis-Menten plot for the effect of increasing concentration of ABTS on the velocity of free Cyt C@Cu-PMOF in water. The reactions were performed with 2 mM ABTS, 0.1-2.2 mM H_2O_2, 5 mM enzyme room temperature.

Table S8. Kinetic parameters of enzymes and enzyme@Cu-POMCOFs in acid-sodium citrate buffer.

	K_m	V_{max}	V_{max}/K_m
Free MP-11	0.57	0.11	0.19
MP-11@Cu-POMCOF	0.73	0.12	0.16
Free Cyt c	0.83	0.089	0.10
Cyt c@Cu-POMCOF	0.93	0.097	0.11

Table S9. Kinetic parameters of MP-11 and MP-11@Cu-POMCOF in water.

	K_m	V_{max}	V_{max}/K_m
Free MP-11	1.92	0.06	0.031
MP-11@Cu-POMCOF	1.43	0.14	0.097

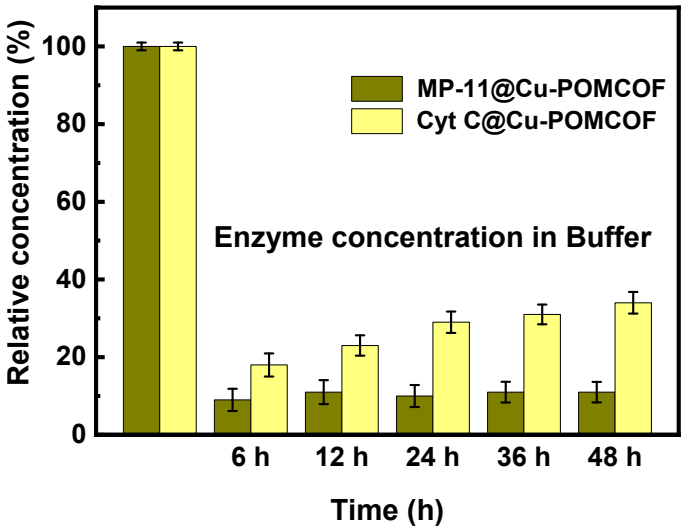

Fig. S12. the recyclability of immobilized enzymes by a simple centrifugation process.

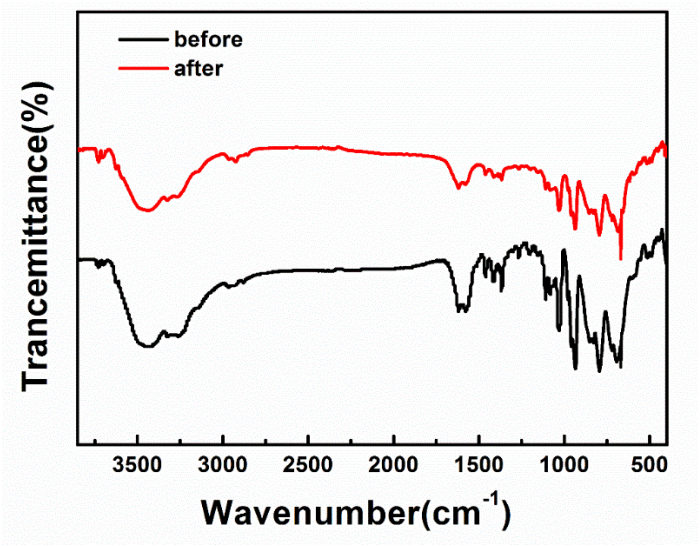

Fig. S13. IR spectra of Cu-POMCOF before and after enzyme encapsulate.