Supporting Information

Polypyrrole Coating Eightfold Helical Wells-Dawson POMs based Cu-FKZ Framework for Boosting Colorimetric Sensing

Qian Li,[a,b] Mingqi Xu,[a,b] Xiao Li,[a] Shuxian Li,[b] Liran Hou,[a] Yuhao Chen,[a] Jingquan Sha*[a,b]

[a]Department of Chemistry and Chemical Engineering, Jining University, Qufu 273155, P. R. China.
[b]School of Pharmacy, Jiamusi University, HeilongJiang, Jiamusi, Heilongjiang,154007, P.R. China.

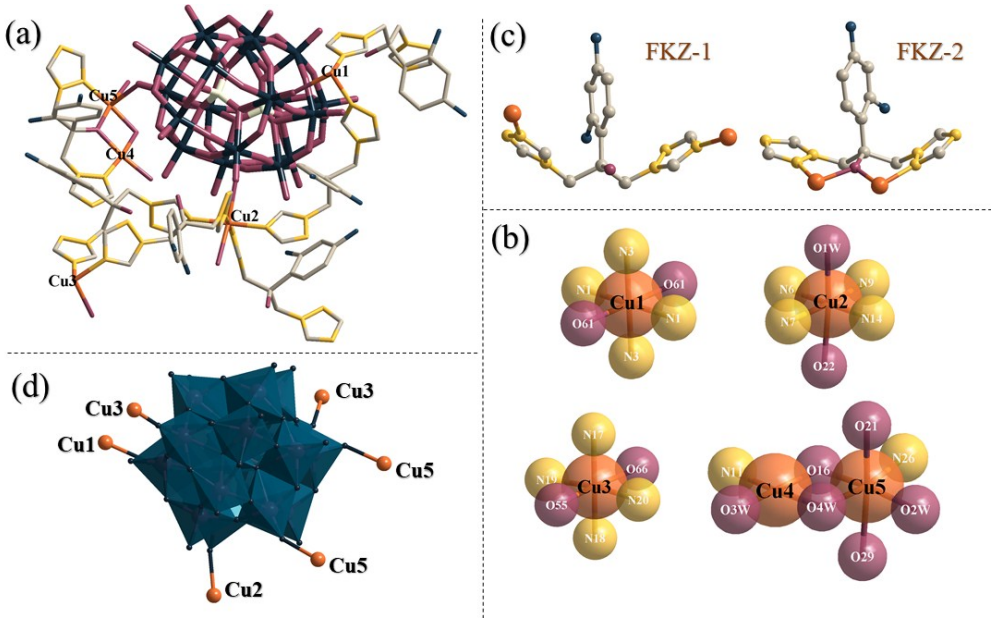


Fig. S1 (a) Combined wires/sticks representation of the asymmetric unit of CuFKZP$_2$W$_{18}$. All the hydrogen atoms and free water molecules have been omitted for clarity; The coordination modes of Cu ions (b) Cu1, Cu2, Cu3, and Cu5 adopt hexadentate coordination modes, and Cu4 adopts tetradentate coordination modes, which are completed by four N from four FKZ-1 and two O from two P_2W_{18}, four N from four FKZ-1 with two O from one P_2W_{18} and one H_2O, four N from four FKZ and two O from two P_2W_{18}, one N from one FKZ with five O from two P_2W_{18}, two H_2O and one FKZ, one N from one FKZ and three O from one FKZ and two H_2O, respectively; (c and d) The coordination modes of the FKZ ligand (c), P_2W_{18} polyanions (d).

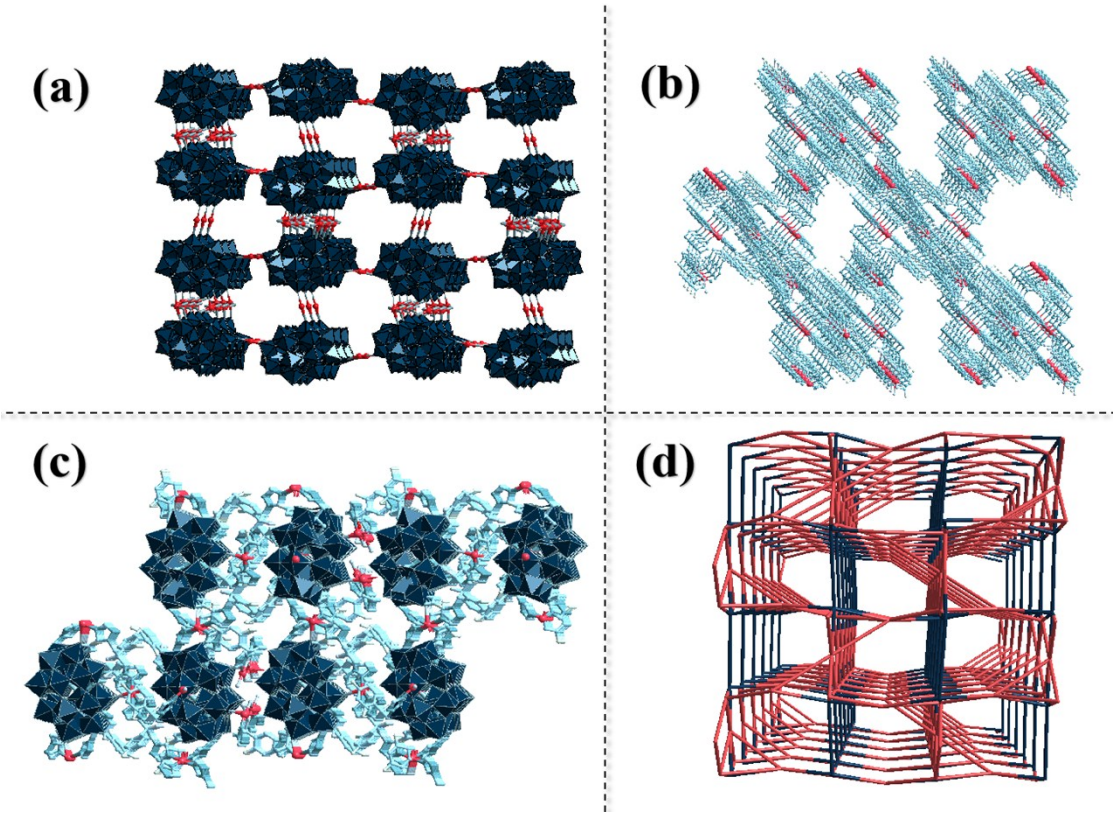


Fig. S2 (a) Ball/stick/polyhedral representation of three-dimensional inorganic backbone containing Type-I meso-helices. (b) Ball/stick representation of three-dimensional inorganic backbone containing Type-II meso-helices. (c) Ball/stick/polyhedral representation of whole three-dimensional framework of $CuFKZP_2W_{18}$ containing Type-I and Type-II meso-helices and FKZ-2. (d) The topology of $Cu(FKZ)P_2W_{18}$ along *a* axis. The dark blue nodes represent P_2W_{18} polyanions, and the burnt-orange nodes symbolize Cu^{2+} ions.

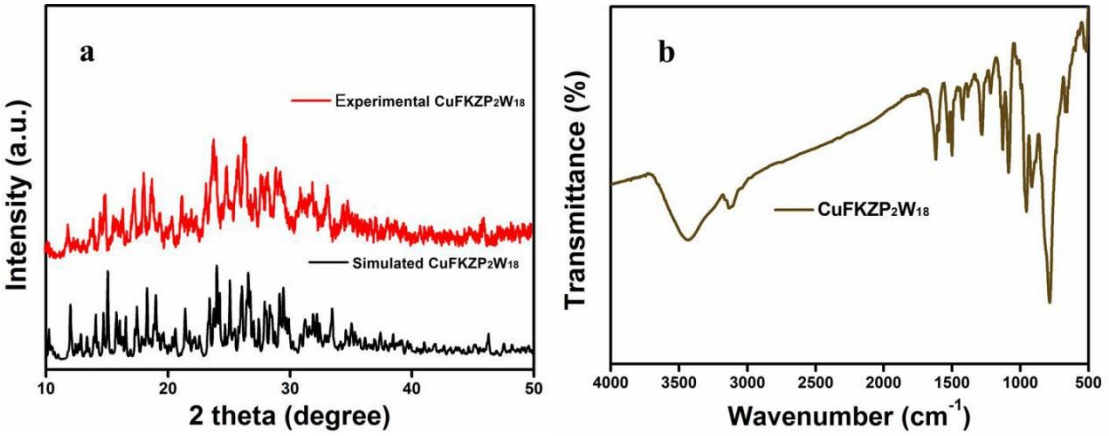


Fig. S3 PXRD patterns (a) and IR spectra (b) of $CuFKZP_2W_{18}$.

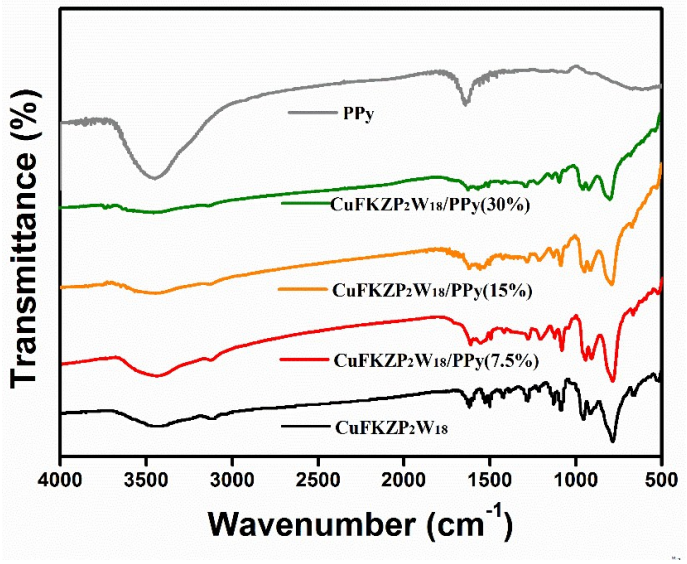


Fig. S4 IR spectra of PPy, $CuFKZP_2W_{18}$ and $CuFKZP_2W_{18}$/PPy(n).

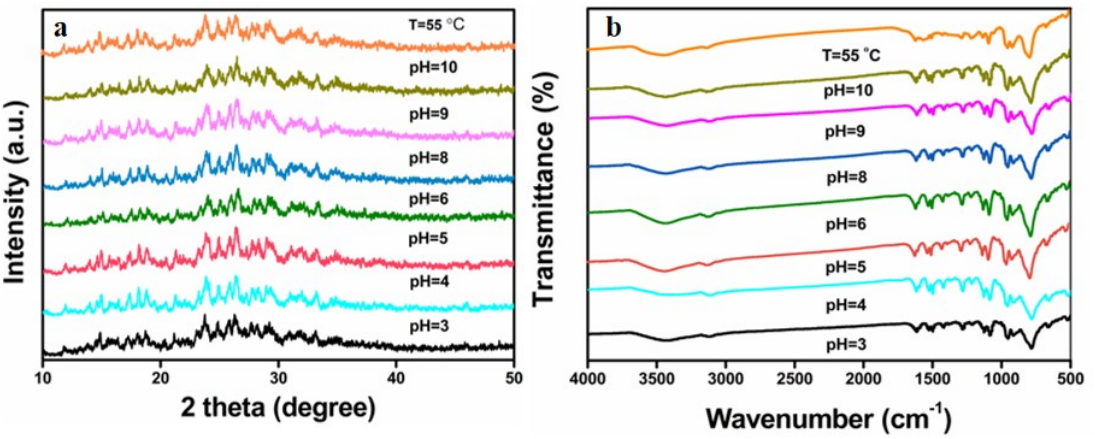


Fig. S5 PXRD patterns (a) and IR spectra (b) of $CuFKZP_2W_{18}$ soaked in aqueous solution with different pH values at room temperature for 12 h and treated at 55°C for 12 h.

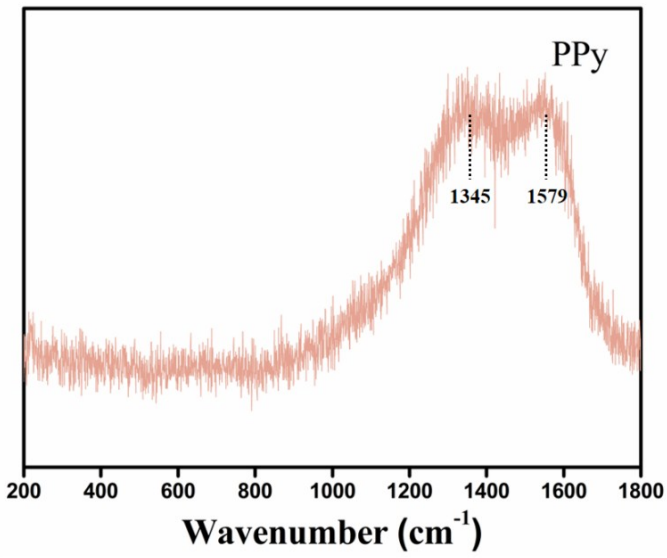


Fig. S6 Raman spectra of PPy.

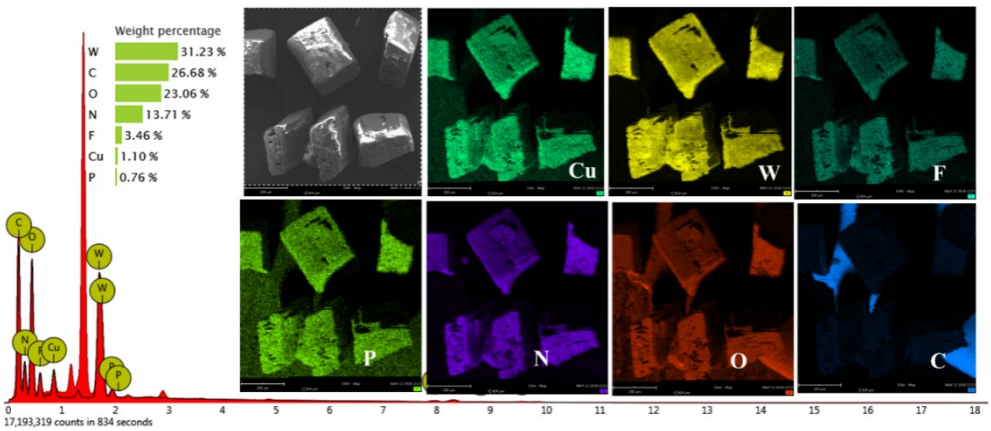


Fig. S7 The corresponding mapping images of C, O,W, P, F, Cu, and N in $CuFKZP_2W_{18}$.

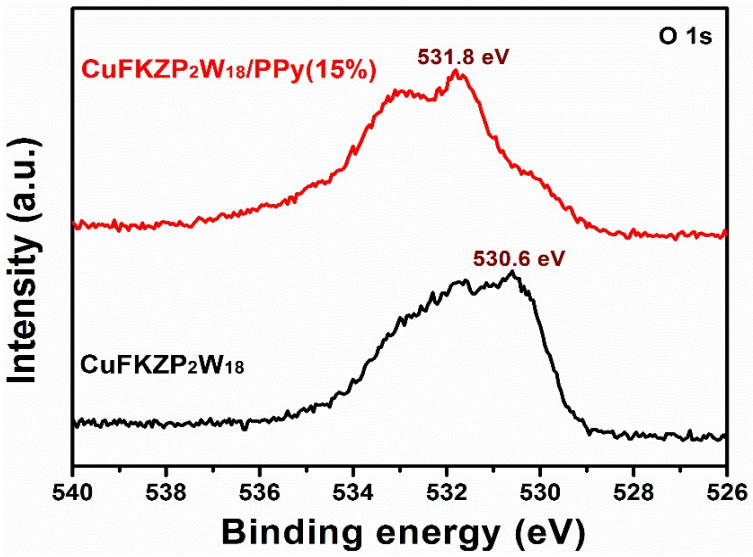


Fig. S8. The O 1s XPS spectra of $CuFKZP_2W_{18}$ and $CuFKZP_2W_{18}$/PPy(15%).

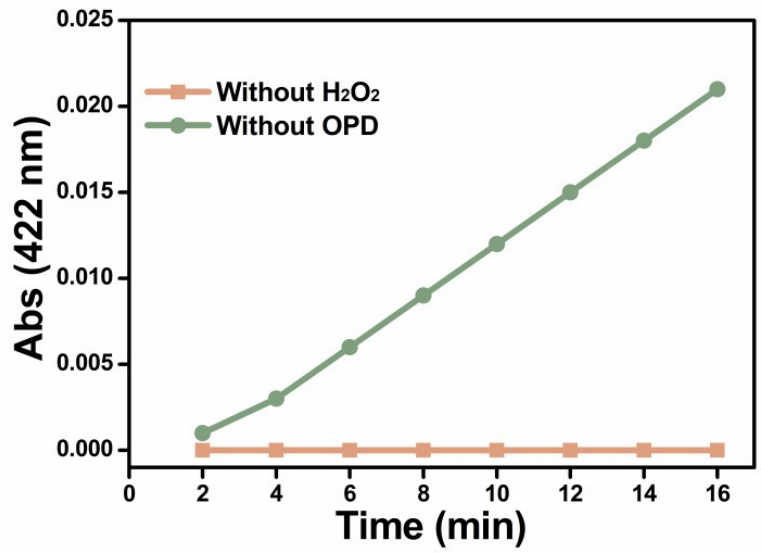


Fig. S9 Time-dependent absorbance of $CuFKZP_2W_{18}$ (0.6 mg/mL) in the absence of H_2O_2 or OPD. Typical reaction conditions: acetate buffer solution (pH=7), H_2O_2 100 μM, OPD 30 μM and 4 min at 40°C.

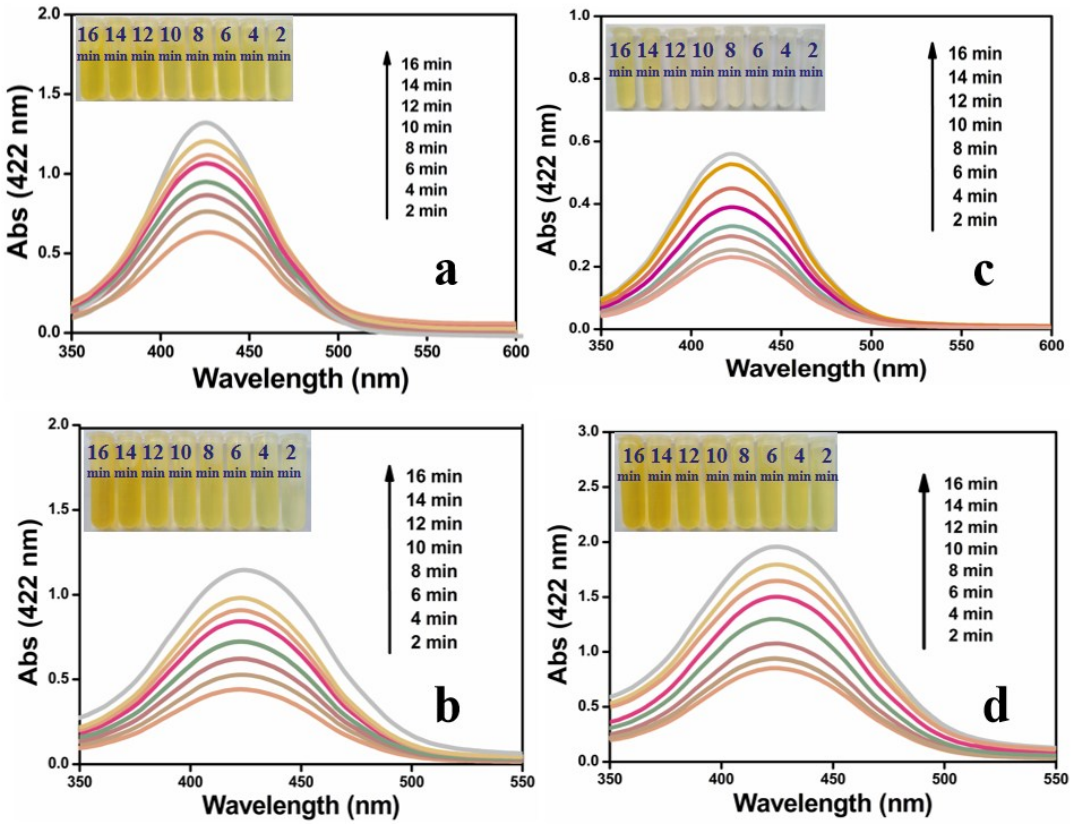


Fig. S10 UV-vis absorption spectra of $CuFKZP_2W_{18}$ (a), $CuFKZP_2W_{18}$/PPy(7%) (b), PPy (c) and $CuFKZP_2W_{18}$/PPy(30%) (d) catalyzed OPD colorimetric system as a functin of reaction time from 2 to 16 min. Typical reaction conditions: $CuFKZP_2W_{18}$/PPy(n%) (0.6 mg/mL), acetate buffer solution (pH=7), H_2O_2 100 μM, OPD 30 μM at 40 °C.

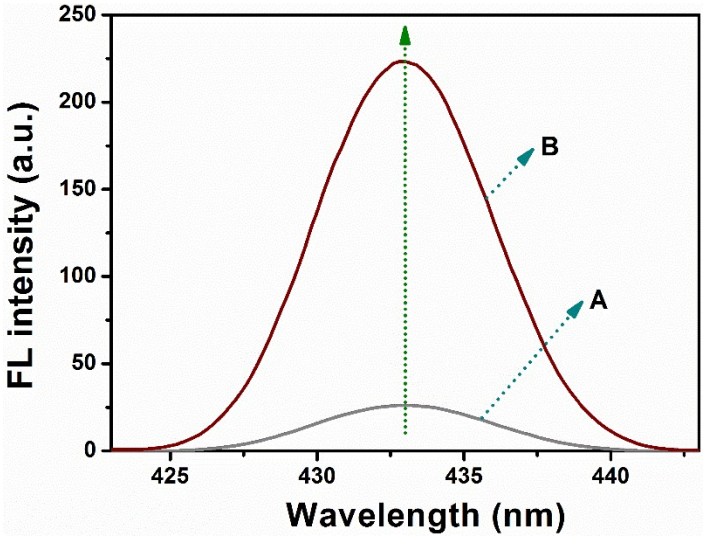


Fig. S11 The corresponding fluorescence spectra of TA solution (2×10^{-3} M) in the absence (A) and presence (B) of $CuFKZP_2W_{18}$/PPy(15%) with H_2O_2 (50 mM) during photoluminescence probing, respectively.

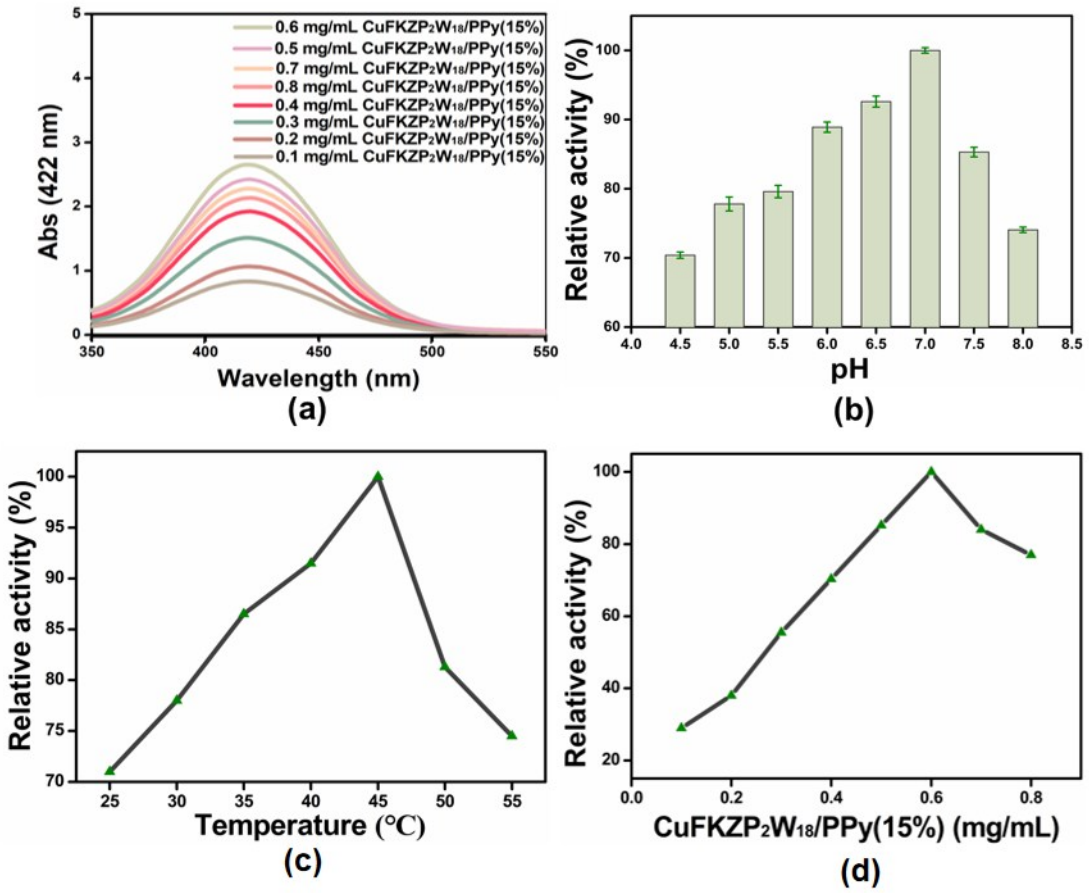


Fig. S12 UV-vis absorption spectra of $CuFKZP_2W_{18}$/PPy(15%) catalyzed OPD colorimetric system as a function of $CuFKZP_2W_{18}$/PPy(15%) dosage (a), reaction acidity (b) and reaction temperature (c). (d) Dependence of the peroxidase-like activity on $CuFKZP_2W_{18}$/PPy(15%) dosage (dosage: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8 mg/mL). Typical reaction conditions: H_2O_2 100 μM, OPD 30 μM, time 4 min and temperature 40 °C.

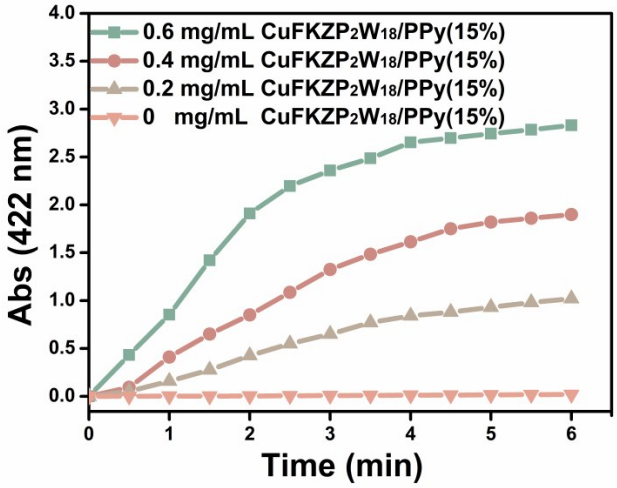


Fig. S13 Time-dependent absorbance changes at 422 nm in the presence of 0 mg/mL, 0.2 mg/mL, 0.4 mg/mL, and 0.6 mg/mL $CuFKZP_2W_{18}$/PPy(15%) in buffer solution (pH 7.0). Typical reaction conditions: H_2O_2 100 μM, OPD 30 μM, time 4 min and temperature 40 °C.

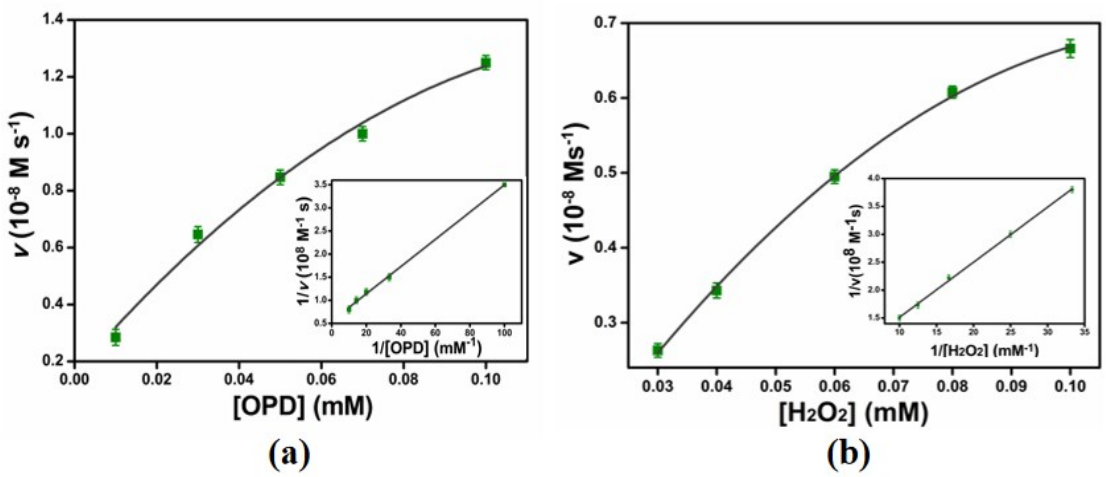


Fig. S14 Steady-state kinetic assays of $CuFKZP_2W_{18}$ (0.6 mg/mL): (a) 100 μM H_2O_2 with varying OPD concentration, (b) 30 μM OPD with varying H_2O_2 concentration. The reaction was performed in pH=7.0 buffer solution, time 4 min and temperature 40 °C.

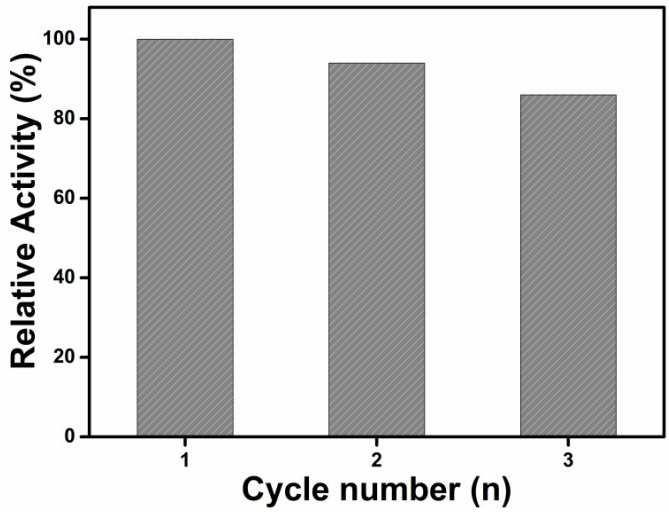


Fig. S15 Reusability of $CuFKZP_2W_{18}$/PPy(15%) (0.6 mg/mL) after repeated cycles. Typical reaction conditions: acetate buffer solution (pH=7), H_2O_2 100 μM, OPD 30 μM, time 4 min and temperature 40 °C.

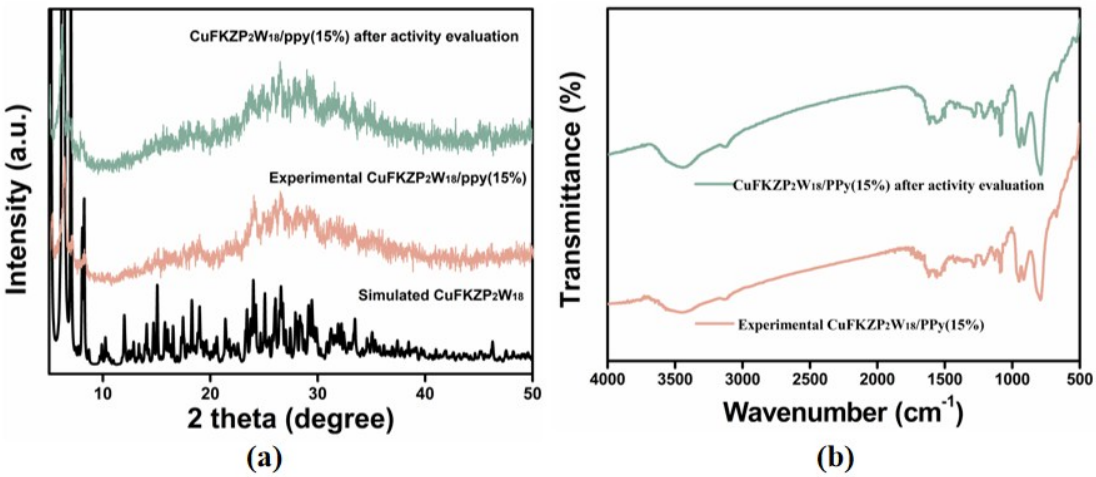
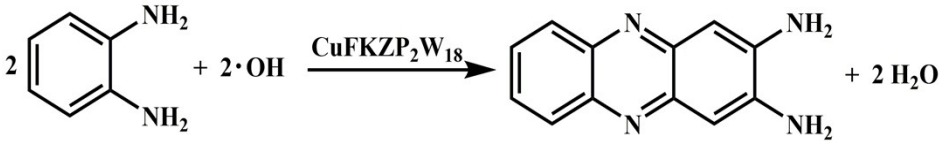
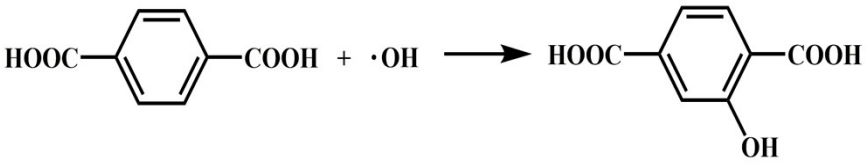


Fig. S16 (a) PXRD patterns of simulated $CuFKZP_2W_{18}$ and $CuFKZP_2W_{18}$/PPy(15%) before and after peroxidase-like activity evaluation. (b) IR spectra of experimental $CuFKZP_2W_{18}$/PPy(15%) and $CuFKZP_2W_{18}$/PPy(15%) after activity evaluation.

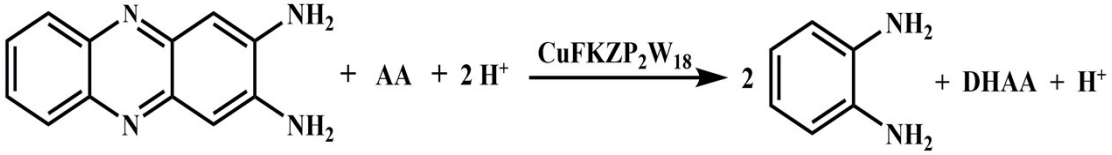


Scheme S1. The oxidation reaction of OPD catalyzed by $CuFKZP_2W_{18}$ in the presence of H_2O_2.



Non-fluorescence **High fluorescence**

Scheme S2. Hydroxyl radicals (·OH) induced the conversion of non-fluorescent terephthalic acid to highly fluorescent 2-hydroxyterephthalic acid.



Scheme S3. AA induced the conversion of oxOPD to OPD.

Table S1. The BVS calculations of W and Cu atoms in $CuFKZP_2W_{18}$ (BL= bond length, BV= bond valence).

BL for W1	**1.713 (O29)**	**1.866 (O30)**	**1.927 (O40)**	**1.867 (O45)**	**1.935 (O47)**	**2.317 (O59)**	
BL for W2	**1.898 (O2)**	**2.356 (O16)**	**1.911 (O19)**	**1.887 (O20)**	**1.875 (O32)**	**1.714 (O61)**	
BL for W3	**2.311 (O6)**	**1.894 (O8)**	**1.933 (O20)**	**1.704 (O22)**	**1.948 (O23)**	**1.855 (O31)**	
BL for W4	**1.697 (O1)**	**1.881 (O2)**	**2.334 (O3)**	**1.906 (O10)**	**1.893 (O18)**	**1.933 (O33)**	
BL for W5	**2.517 (O6)**	**1.874 (O8)**	**1.926 (O10)**	**1.883 (O15)**	**1.658 (O16)**	**1.894 (O23)**	
BL for W6	**2.369 (O9)**	**1.913 (O15)**	**1.868 (O23)**	**1.709 (O24)**	**1.901 (O25)**	**1.908 (O27)**	
BL for W7	**1.917 (O35)**	**1.914 (O40)**	**1.876 (O48)**	**1.912 (O54)**	**2.349 (O59)**	**1.690 (O60)**	
BL for W8	**2.342 (O5)**	**1.879 (O12)**	**1.905 (O0AA)**	**1.924 (O1AA)**	**1.713 (O21)**	**1.900 (O35)**	
BL for W9	**1.940 (O31)**	**2.376 (O36)**	**1.926 (O42)**	**1.889 (O43)**	**1.699 (O44)**	**1.904 (O45)**	

BL for W10	**2.367 (O5)**	**1.878 (O8)**	**1.919 (O0AA)**	**1.693 (O14)**	**1.881 (O15)**	**1.953 (O30)**	
BL for W11	**1.688 (O4)**	**1.912 (O32)**	**2.377 (O36)**	**1.899 (O41)**	**1.905 (O42)**	**1.909 (O46)**	
BL for W12	**2.409 (O9)**	**1.910 (O18)**	**1.895 (O19)**	**1.926 (O25)**	**1.665 (O26)**	**1.906 (O28)**	
BL for W13	**1.693 (O7)**	**1.860 (O33)**	**2.344 (O38)**	**1.875 (O41)**	**1.899 (O56)**	**1.933 (O62)**	
BL for W14	**2.352 (O37)**	**1.889 (O46)**	**1.913 (O49)**	**1.903 (O50)**	**1.697 (O55)**	**1.874 (O62)**	
BL for W15	**2.373 (O37)**	**1.902 (O43)**	**1.899 (O47)**	**1.911 (O49)**	**1.687 (O51)**	**1.899 (O52)**	
BL for W16	**1.917 (O9)**	**1.914 (O1AA)**	**1.876 (O17)**	**1.912 (O27)**	**2.349 (O28)**	**1.713 (O66)**	
BL for W17	**1.886 (O3)**	**2.374 (O10)**	**1.925 (O11)**	**1.886 (O12)**	**1.691 (O17)**	**1.920 (O34)**	
BL for W18	**2.387 (O37)**	**1.903 (O50)**	**1.927 (O52)**	**1.684 (O53)**	**1.897 (O54)**	**1.887 (O57)**	
BL for Cu1	**2.481 (O61)**	**2.481 (O61)**	**2.015 (N1)**	**2.015 (N1)**	**2.009 (N3)**	**2.009 (N3)**	
BL for Cu2	**2.316 (O22)**	**2.286 (N103)**	**2.013 (N6)**	**2.038 (N7)**	**1.995 (N9)**	**2.005 (N14)**	
BL for Cu3	**2.595 (O55)**	**2.301 (O66)**	**1.992 (N17)**	**2.014 (O18)**	**2.002 (N19)**	**1.999 (N20)**	
BL for Cu4	**1.902 (O16)**	**2.861 (O40)**	**1.939 (O58)**	**1.916 (O102)**	**1.938 (N11)**		
BL for Cu5	**2.141 (O13)**	**1.941 (O16)**	**2.447 (O21)**	**2.559 (O29)**	**1.971 (O102)**	**1.956 (N26)**	
BV for W1	**1.9224**	**1.1131**	**0.8952**	**1.1091**	**0.8700**	**0.2223**	**6.1321 (total)**
BV for W2	**0.9929**	**0.1934**	**0.9478**	**1.0327**	**1.0779**	**1.9155**	**6.1602 (total)**
BV for W3	**0.2272**	**1.0072**	**0.8762**	**1.9852**	**0.8305**	**1.1577**	**6.0839 (total)**
BV for W4	**2.0354**	**1.0550**	**0.2092**	**0.9649**	**1.0108**	**0.8762**	**6.1516 (total)**
BV for W5	**0.1088**	**1.0817**	**0.8984**	**1.0475**	**2.3396**	**1.0072**	**6.4833 (total)**
BV for W6	**0.1847**	**0.9411**	**1.1052**	**1.9501**	**0.9823**	**0.9580**	**6.1213 (total)**
BV for W7	**0.9277**	**0.9377**	**1.0740**	**0.9445**	**0.1983**	**2.0870**	**6.1693 (total)**
BV for W8	**0.2033**	**1.0626**	**0.9684**	**0.9048**	**1.9224**	**0.9858**	**6.0474 (total)**
BV for W9	**0.8546**	**0.1801**	**0.8984**	**1.0253**	**2.0210**	**0.9718**	**5.9512 (total)**
BV for W10	**0.1860**	**1.0664**	**0.9211**	**2.0647**	**1.0550**	**0.8158**	**6.1091 (total)**
BV for W11	**2.1019**	**0.9445**	**0.1795**	**0.9893**	**0.9684**	**0.9546**	**6.1382 (total)**
BV for W12	**0.1601**	**0.9512**	**1.0036**	**0.8984**	**2.2819**	**0.9649**	**6.2601 (total)**
BV for W13	**2.0647**	**1.1372**	**0.2019**	**1.0779**	**0.9893**	**0.8762**	**6.3473 (total)**
BV for W14	**0.1962**	**1.0253**	**0.9411**	**0.9753**	**2.0354**	**1.0817**	**6.2551 (total)**
BV for W15	**0.1820**	**0.9788**	**0.9893**	**0.9478**	**2.1095**	**0.9893**	**6.1968 (total)**

BV for W16	**0.9277**	**0.9377**	**1.0740**	**0.9445**	**0.1983**	**1.9224**	**6.0046 (total)**
BV for W17	**1.0364**	**0.1814**	**0.9016**	**1.0364**	**2.0795**	**0.9179**	**6.1531 (total)**
BV for W18	**0.1732**	**0.9753**	**0.8952**	**2.1322**	**0.9964**	**1.0327**	**6.2049 (total)**
BV for Cu1	**0.1073**	**0.1073**	**0.4221**	**0.4221**	**0.4493**	**0.4493**	**1.9974 (total)**
BV for Cu2	**0.1675**	**0.2125**	**0.4445**	**0.4155**	**0.4667**	**0.4542**	**2.1893 (total)**
BV for Cu3	**0.0788**	**0.1745**	**0.4705**	**0.3790**	**0.4579**	**0.4616**	**2.0223 (total)**
BV for Cu4	**0.5130**	**0.0384**	**0.4641**	**0.4939**	**0.5444**		**2.0538 (total)**
BV for Cu5	**0.2689**	**0.4616**	**0.1176**	**0.0869**	**0.4257**	**0.5185**	**1.8792 (total)**

Table S2. Selected bond lengths (Å) and bond angles (°) for $CuFKZP_2W_{18}$.

Bond	Lengths	Bond	Lengths
C(1)-N(7)	1.32(2)	O(3)-W(17)	2.373(10)
C(1)-N(8)	1.33(2)	O(4)-W(11)	1.689(11)
C(2)-N(2)	1.33(3)	O(5)-P(1)	1.513(11)
C(2)-N(7)	1.35(3)	O(5)-W(8)	2.342(10)
C(3)-N(4)	1.35(3)	O(5)-W(10)	2.367(11)
C(3)-N(19)	1.37(3)	O(6)-P(1)	1.544(10)
C(4)-N(14)	1.33(2)	O(6)-W(3)	2.311(10)
C(4)-N(22)	1.35(2)	O(6)-W(2)	2.355(10)
C(5)-N(25)	1.32(3)	O(7)-W(13)	1.692(11)
C(5)-N(31)	1.35(4)	O(8)-W(10)	1.877(10)
C(6)-N(10)	1.32(2)	O(8)-W(3)	1.895(10)
C(6)-N(9)	1.32(2)	O(9)-P(1)	1.584(10)
N(40)-C(44)	1.30(3)	O(9)-W(16)	2.321(10)
N(40)-N(10)	1.37(2)	O(9)-W(6)	2.371(11)
C(8)-N(10)	1.47(3)	O(9)-W(12)	2.408(10)
C(8)-C(74)	1.51(3)	O(10)-W(5)	1.905(11)
C(9)-C(17)	1.3900	O(10)-W(17)	1.921(11)
C(9)-C(69)	1.3900	O(11)-W(17)	1.692(11)
C(17)-C(87)	1.3900	O(12)-W(8)	1.878(11)
C(17)-F(13A)	1.50(4)	O(12)-W(17)	1.887(11)
C(17)-F(13B)	1.52(6)	O(0AA)-W(8)	1.905(12)
C(87)-C(24)	1.3900	O(0AA)-W(10)	1.919(11)
C(24)-C(68)	1.3900	O(14)-W(10)	1.693(11)
C(68)-C(69)	1.3900	O(15)-W(10)	1.882(10)
C(68)-C(54)	1.58(3)	O(15)-W(6)	1.912(10)
C(69)-F(2)	1.29(2)	O(1AA)-W(16)	1.882(10)
C(10)-N(8)	1.48(2)	O(1AA)-W(8)	1.923(10)
C(10)-C(54)	1.52(3)	O(17)-W(16)	1.890(11)
C(11)-N(21)	1.46(2)	O(17)-W(17)	1.924(10)

C(11)-C(45)	1.56(2)	O(18)-W(5)	1.894(11)
C(12)-N(29)	1.29(3)	O(18)-W(12)	1.910(11)
C(12)-N(21)	1.33(2)	O(19)-W(12)	1.895(10)
C(18)-N(5)	1.32(2)	O(19)-W(2)	1.911(10)
C(18)-N(6)	1.33(2)	O(20)-W(2)	1.886(10)
C(19)-N(35)	1.32(2)	O(20)-W(3)	1.933(10)
C(19)-N(6)	1.35(2)	O(21)-W(8)	1.713(10)
C(21)-N(5)	1.47(2)	O(22)-W(3)	1.703(11)
C(21)-C(45)	1.55(2)	O(22)-Cu(2)	2.317(11)
C(25)-C(27)	1.32(4)	O(23)-W(6)	1.867(10)
C(25)-C(83)	1.43(3)	O(23)-W(3)	1.949(10)
C(26)-C(27)	1.36(4)	O(24)-W(6)	1.708(11)
C(26)-C(85)	1.43(3)	O(25)-W(6)	1.901(11)
C(27)-F(10)	1.38(3)	O(25)-W(12)	1.927(11)
C(28)-N(11)	1.34(3)	O(26)-W(12)	1.664(12)
C(28)-N(24)	1.37(3)	O(27)-W(6)	1.907(11)
C(31)-N(23)	1.46(2)	O(27)-W(16)	1.908(11)
C(31)-C(32)	1.57(3)	O(28)-W(12)	1.906(11)
C(32)-O(16)	1.408(19)	O(28)-W(16)	1.926(11)
C(32)-C(34)	1.52(2)	O(29)-W(1)	1.712(11)
C(32)-C(48)	1.56(3)	O(30)-W(1)	1.867(10)
C(33)-C(76)	1.37(3)	O(30)-W(10)	1.955(10)
C(33)-C(34)	1.38(3)	O(31)-W(3)	1.856(10)
C(34)-C(66)	1.38(2)	O(31)-W(9)	1.940(10)
C(39)-N(22)	1.49(2)	O(32)-W(2)	1.874(10)
C(39)-C(40)	1.54(3)	O(32)-W(11)	1.913(10)
C(40)-O(64)	1.42(2)	O(33)-W(13)	1.861(11)
C(40)-C(75)	1.52(3)	O(33)-W(5)	1.933(11)
C(40)-C(41)	1.55(3)	O(34)-W(17)	1.887(11)
C(41)-N(27)	1.47(2)	O(34)-W(4)	1.894(11)
C(42)-C(80)	1.42(4)	O(35)-W(8)	1.902(10)
C(42)-C(82)	1.47(5)	O(35)-W(7)	1.915(10)
C(43)-N(15)	1.31(2)	O(36)-P(2)	1.505(10)
C(43)-N(14)	1.36(2)	O(36)-W(9)	2.377(10)
C(44)-N(9)	1.34(2)	O(36)-W(11)	2.378(10)
C(45)-O(63)	1.418(18)	O(37)-P(2)	1.586(10)
C(45)-C(84)	1.50(2)	O(37)-W(14)	2.352(10)
C(46)-N(26)	1.33(3)	O(37)-W(15)	2.374(11)

C(46)-N(31)	1.38(4)	O(37)-W(18)	2.388(10)
C(47)-N(23)	1.34(3)	O(38)-P(2)	1.540(11)
C(47)-N(24)	1.38(3)	O(38)-W(13)	2.343(11)
C(48)-N(25)	1.44(3)	O(38)-W(4)	2.362(11)
C(49)-N(21)	1.33(2)	O(39)-W(4)	1.681(11)
C(49)-N(1)	1.33(2)	O(40)-W(7)	1.914(11)
O(13)-Cu(5)	2.14(3)	O(40)-W(1)	1.926(11)
C(52)-N(19)	1.33(2)	O(41)-W(13)	1.875(11)
C(52)-N(28)	1.34(3)	O(41)-W(11)	1.899(11)
C(53)-C(54)	1.50(3)	O(42)-W(11)	1.906(10)
C(53)-N(28)	1.50(3)	O(42)-W(9)	1.929(10)
C(54)-O(65)	1.41(2)	O(43)-W(9)	1.887(10)
C(55)-N(27)	1.31(2)	O(43)-W(15)	1.904(11)
C(55)-N(18)	1.36(2)	O(44)-W(9)	1.699(11)
N(39)-C(117)	1.35(3)	O(45)-W(1)	1.868(10)
N(39)-N(27)	1.38(2)	O(45)-W(9)	1.903(11)
C(57)-N(17)	1.33(2)	O(46)-W(14)	1.889(10)
C(57)-N(58)	1.35(3)	O(46)-W(11)	1.909(10)
N(58)-N(59)#1	1.32(2)	O(47)-W(15)	1.900(10)
N(59)-N(58)#2	1.32(2)	O(47)-W(1)	1.934(10)
N(59)-C(60)#2	1.35(3)	O(48)-W(7)	1.874(11)
N(59)-C(72)	1.49(3)	O(48)-W(4)	1.878(11)
C(60)-N(17)	1.31(2)	O(49)-W(15)	1.911(11)
C(60)-N(59)#1	1.35(3)	O(49)-W(14)	1.912(12)
C(61)-N(36)	1.30(3)	O(50)-W(18)	1.903(10)
C(61)-N(3)	1.36(2)	O(50)-W(14)	1.903(10)
C(62)-N(3)	1.30(2)	O(51)-W(15)	1.687(12)
C(62)-N(30)	1.31(2)	O(52)-W(15)	1.899(12)
C(66)-C(78)	1.36(3)	O(52)-W(18)	1.927(12)
C(66)-F(3)	1.38(3)	O(53)-W(18)	1.684(11)
O(99)-C(74)	1.46(3)	O(54)-W(18)	1.896(11)
C(72)-C(74)	1.58(3)	O(54)-W(7)	1.913(11)
C(74)-C(106)	1.50(3)	O(55)-W(14)	1.696(11)
C(75)-C(79)	1.37(3)	O(56)-W(13)	1.898(11)
C(75)-C(80)	1.46(3)	O(56)-W(4)	1.911(11)
C(76)-C(77)	1.38(4)	O(57)-W(18)	1.887(11)
C(77)-C(78)	1.33(4)	O(57)-W(4)	1.947(10)
C(77)-F(4)	1.37(2)	O(58)-Cu(4)	1.939(12)

C(79)-F(5)	1.31(3)	O(59)-P(2)	1.545(11)
C(79)-C(81)	1.41(3)	O(59)-W(1)	2.318(11)
C(81)-C(82)	1.36(4)	O(59)-W(7)	2.350(10)
C(82)-F(7)	1.37(3)	O(60)-W(7)	1.690(11)
C(83)-F(1)	1.34(3)	O(61)-W(2)	1.713(10)
C(83)-C(84)	1.35(3)	O(62)-W(14)	1.875(11)
C(84)-C(85)	1.37(3)	O(62)-W(13)	1.932(10)
N(1)-N(29)	1.37(2)	O(66)-W(16)#3	1.713(11)
N(1)-Cu(1)	2.014(13)	O(66)-Cu(3)	2.303(11)
N(2)-N(8)	1.34(2)	Cu(1)-N(3)#4	2.010(14)
N(3)-Cu(1)	2.010(14)	Cu(1)-N(1)#4	2.014(13)
N(4)-N(28)	1.36(2)	Cu(2)-O(103)	2.29(3)
N(5)-N(35)	1.34(2)	Cu(4)-Cu(5)	2.968(3)
N(6)-Cu(2)	2.014(14)	W(16)-O(66)#5	1.712(11)
N(7)-Cu(2)	2.039(15)	C(101)-C(103)	1.3900
N(9)-Cu(2)	1.995(14)	C(101)-C(106)	1.3900
N(11)-N(23)	1.37(2)	C(103)-C(105)	1.3900
N(11)-Cu(4)	1.938(17)	C(105)-F(8)	1.37(4)
O(102)-Cu(4)	1.916(12)	C(105)-C(102)	1.3900
O(102)-Cu(5)	1.972(12)	C(102)-C(104)	1.3900
N(14)-Cu(2)	2.006(14)	C(104)-C(106)	1.3900
N(15)-N(22)	1.36(2)	C(104)-F(9)	1.45(3)
O(16)-Cu(4)	1.900(12)	O(100)-C(7)	1.38(3)
O(16)-Cu(5)	1.941(12)	C(7)-C(111)	1.47(3)
N(17)-Cu(3)	1.992(14)	C(7)-C(118)	1.54(3)
N(18)-C(117)	1.34(3)	C(7)-C(120)	1.55(4)
N(18)-Cu(3)	2.014(16)	N(100)-N(101)	1.26(3)
N(19)-Cu(3)	2.002(16)	N(100)-C(119)	1.36(4)
N(20)-C(119)	1.33(3)	C(120)-N(101)#6	1.52(4)
N(20)-C(121)	1.40(3)	C(121)-N(101)	1.35(3)
N(20)-Cu(3)	1.999(18)	N(101)-C(120)#7	1.52(4)
N(25)-N(26)	1.37(2)	C(111)-C(116)	1.3900
N(26)-Cu(5)	1.957(19)	C(111)-C(114)	1.3900
N(30)-N(36)	1.37(2)	C(116)-C(115)	1.3900
N(30)-C(118)	1.46(3)	C(116)-F(12)	1.41(4)
O(1)-W(5)	1.698(11)	C(115)-C(113)	1.3900
O(2)-W(5)	1.881(9)	C(113)-F(11)	1.366(17)
O(2)-W(2)	1.898(10)	C(113)-C(112)	1.3900

O(3)-P(1)	1.527(11)	C(112)-C(114)	1.3900
O(3)-W(5)	2.335(10)	F(13A)-F(13B)	1.37(6)

Bond	**Angles**	**Bond**	**Angles**
N(7)-C(1)-N(8)	109.5(17)	O(16)-Cu(5)-O(102)	78.5(5)
N(2)-C(2)-N(7)	111.6(19)	N(26)-Cu(5)-O(102)	168.8(7)
N(4)-C(3)-N(19)	113.6(19)	O(16)-Cu(5)-O(13)	172.8(7)
N(14)-C(4)-N(22)	109.5(16)	N(26)-Cu(5)-O(13)	95.6(8)
N(25)-C(5)-N(31)	107(3)	O(102)-Cu(5)-O(13)	94.7(6)
N(10)-C(6)-N(9)	111.1(16)	O(16)-Cu(5)-Cu(4)	38.9(3)
C(44)-N(40)-N(10)	103.9(17)	N(26)-Cu(5)-Cu(4)	130.2(6)
N(10)-C(8)-C(74)	111.3(19)	O(102)-Cu(5)-Cu(4)	39.6(4)
C(17)-C(9)-C(69)	120.0	O(13)-Cu(5)-Cu(4)	134.2(5)
C(87)-C(17)-C(9)	120.0	O(29)-W(1)-O(30)	99.3(5)
C(87)-C(17)-F(13A)	124(3)	O(29)-W(1)-O(45)	104.4(5)
C(9)-C(17)-F(13A)	113(3)	O(30)-W(1)-O(45)	89.7(4)
C(87)-C(17)-F(13B)	114(3)	O(29)-W(1)-O(40)	97.1(5)
C(9)-C(17)-F(13B)	113(3)	O(30)-W(1)-O(40)	90.9(4)
F(13A)-C(17)-F(13B)	54(2)	O(45)-W(1)-O(40)	158.1(5)
C(24)-C(87)-C(17)	120.0	O(29)-W(1)-O(47)	96.4(5)
C(87)-C(24)-C(68)	120.0	O(30)-W(1)-O(47)	164.3(4)
C(69)-C(68)-C(24)	120.0	O(45)-W(1)-O(47)	85.3(4)
C(69)-C(68)-C(54)	118.5(18)	O(40)-W(1)-O(47)	88.2(4)
C(24)-C(68)-C(54)	121.3(18)	O(29)-W(1)-O(59)	170.4(5)
F(2)-C(69)-C(68)	122.1(19)	O(30)-W(1)-O(59)	83.8(4)
F(2)-C(69)-C(9)	117.7(19)	O(45)-W(1)-O(59)	84.6(4)
C(68)-C(69)-C(9)	120.0	O(40)-W(1)-O(59)	73.7(4)
N(8)-C(10)-C(54)	107.8(15)	O(47)-W(1)-O(59)	80.9(4)
N(21)-C(11)-C(45)	109.8(13)	O(61)-W(2)-O(32)	97.9(5)
N(29)-C(12)-N(21)	102.9(16)	O(61)-W(2)-O(20)	101.6(5)
N(5)-C(18)-N(6)	109.7(15)	O(32)-W(2)-O(20)	91.2(4)
N(35)-C(19)-N(6)	113.4(17)	O(61)-W(2)-O(2)	100.9(5)
N(5)-C(21)-C(45)	109.5(14)	O(32)-W(2)-O(2)	88.2(4)
C(27)-C(25)-C(83)	114(2)	O(20)-W(2)-O(2)	157.3(4)
C(27)-C(26)-C(85)	116(2)	O(61)-W(2)-O(19)	97.6(5)
C(25)-C(27)-C(26)	128(2)	O(32)-W(2)-O(19)	164.2(4)
C(25)-C(27)-F(10)	117(3)	O(20)-W(2)-O(19)	88.4(4)
C(26)-C(27)-F(10)	115(3)	O(2)-W(2)-O(19)	86.1(4)
N(11)-C(28)-N(24)	112(2)	O(61)-W(2)-O(6)	174.8(5)

N(23)-C(31)-C(32)	110.4(14)	O(32)-W(2)-O(6)	82.6(4)
O(16)-C(32)-C(34)	111.3(14)	O(20)-W(2)-O(6)	73.2(4)
O(16)-C(32)-C(48)	108.2(15)	O(2)-W(2)-O(6)	84.2(4)
C(34)-C(32)-C(48)	113.7(16)	O(19)-W(2)-O(6)	82.2(4)
O(16)-C(32)-C(31)	108.0(15)	O(22)-W(3)-O(31)	98.3(5)
C(34)-C(32)-C(31)	111.3(15)	O(22)-W(3)-O(8)	99.7(5)
C(48)-C(32)-C(31)	103.9(14)	O(31)-W(3)-O(8)	88.8(4)
C(76)-C(33)-C(34)	123(2)	O(22)-W(3)-O(20)	101.9(5)
C(33)-C(34)-C(66)	114.0(18)	O(31)-W(3)-O(20)	92.6(4)
C(33)-C(34)-C(32)	122.0(15)	O(8)-W(3)-O(20)	157.9(4)
C(66)-C(34)-C(32)	123.6(18)	O(22)-W(3)-O(23)	95.7(5)
N(22)-C(39)-C(40)	110.1(15)	O(31)-W(3)-O(23)	165.4(4)
O(64)-C(40)-C(75)	109.8(18)	O(8)-W(3)-O(23)	85.1(4)
O(64)-C(40)-C(39)	110.9(15)	O(20)-W(3)-O(23)	88.2(4)
C(75)-C(40)-C(39)	110.3(18)	O(22)-W(3)-O(6)	174.9(5)
O(64)-C(40)-C(41)	105.3(17)	O(31)-W(3)-O(6)	84.1(4)
C(75)-C(40)-C(41)	109.7(17)	O(8)-W(3)-O(6)	84.7(4)
C(39)-C(40)-C(41)	110.8(17)	O(20)-W(3)-O(6)	73.5(4)
N(27)-C(41)-C(40)	109.9(17)	O(23)-W(3)-O(6)	82.2(4)
C(80)-C(42)-C(82)	113(3)	O(39)-W(4)-O(48)	103.9(5)
N(15)-C(43)-N(14)	113.4(19)	O(39)-W(4)-O(34)	98.9(5)
N(40)-C(44)-N(9)	114.1(18)	O(48)-W(4)-O(34)	89.4(5)
O(63)-C(45)-C(84)	106.0(13)	O(39)-W(4)-O(56)	100.2(5)
O(63)-C(45)-C(21)	109.4(13)	O(48)-W(4)-O(56)	155.7(5)
C(84)-C(45)-C(21)	112.3(14)	O(34)-W(4)-O(56)	89.6(5)
O(63)-C(45)-C(11)	107.6(13)	O(39)-W(4)-O(57)	96.6(5)
C(84)-C(45)-C(11)	113.6(14)	O(48)-W(4)-O(57)	86.2(5)
C(21)-C(45)-C(11)	107.7(13)	O(34)-W(4)-O(57)	164.5(4)
N(26)-C(46)-N(31)	110(3)	O(56)-W(4)-O(57)	88.5(4)
N(23)-C(47)-N(24)	108.3(18)	O(39)-W(4)-O(38)	172.0(5)
N(25)-C(48)-C(32)	110.4(16)	O(48)-W(4)-O(38)	84.0(4)
N(21)-C(49)-N(1)	108.3(14)	O(34)-W(4)-O(38)	82.3(4)
N(19)-C(52)-N(28)	109.1(17)	O(56)-W(4)-O(38)	71.8(4)
C(54)-C(53)-N(28)	110.7(19)	O(57)-W(4)-O(38)	82.5(4)
O(65)-C(54)-C(53)	111.6(17)	O(1)-W(5)-O(2)	102.1(5)
O(65)-C(54)-C(10)	111.1(19)	O(1)-W(5)-O(18)	98.6(5)
C(53)-C(54)-C(10)	109.6(19)	O(2)-W(5)-O(18)	86.0(4)
O(65)-C(54)-C(68)	104.4(18)	O(1)-W(5)-O(10)	98.7(5)

C(53)-C(54)-C(68)	113.0(18)	O(2)-W(5)-O(10)	159.1(5)
C(10)-C(54)-C(68)	107.0(16)	O(18)-W(5)-O(10)	92.2(5)
N(27)-C(55)-N(18)	109.2(17)	O(1)-W(5)-O(33)	97.3(5)
C(117)-N(39)-N(27)	102.6(17)	O(2)-W(5)-O(33)	86.9(4)
N(17)-C(57)-N(58)	114.5(16)	O(18)-W(5)-O(33)	163.6(5)
N(59)#1-N(58)-C(57)	101.3(15)	O(10)-W(5)-O(33)	89.2(5)
N(58)#2-N(59)-C(60)#2	111.4(17)	O(1)-W(5)-O(3)	173.2(5)
N(58)#2-N(59)-C(72)	123.0(19)	O(2)-W(5)-O(3)	84.5(4)
C(60)#2-N(59)-C(72)	125.2(19)	O(18)-W(5)-O(3)	83.2(4)
N(17)-C(60)-N(59)#1	108.8(18)	O(10)-W(5)-O(3)	74.7(4)
N(36)-C(61)-N(3)	113.6(19)	O(33)-W(5)-O(3)	81.4(4)
N(3)-C(62)-N(30)	110.5(17)	O(24)-W(6)-O(23)	102.2(5)
C(78)-C(66)-F(3)	115.9(19)	O(24)-W(6)-O(25)	101.3(5)
C(78)-C(66)-C(34)	125(2)	O(23)-W(6)-O(25)	90.3(5)
F(3)-C(66)-C(34)	118(2)	O(24)-W(6)-O(27)	102.0(5)
N(59)-C(72)-C(74)	105.9(18)	O(23)-W(6)-O(27)	155.7(5)
O(99)-C(74)-C(106)	98.7(19)	O(25)-W(6)-O(27)	87.0(5)
O(99)-C(74)-C(8)	108(2)	O(24)-W(6)-O(15)	101.1(5)
C(106)-C(74)-C(8)	118(2)	O(23)-W(6)-O(15)	84.9(4)
O(99)-C(74)-C(72)	109.3(19)	O(25)-W(6)-O(15)	157.6(5)
C(106)-C(74)-C(72)	114.0(19)	O(27)-W(6)-O(15)	88.6(5)
C(8)-C(74)-C(72)	107.3(19)	O(24)-W(6)-O(9)	172.9(5)
C(79)-C(75)-C(80)	117(2)	O(23)-W(6)-O(9)	83.7(4)
C(79)-C(75)-C(40)	122(2)	O(25)-W(6)-O(9)	74.5(4)
C(80)-C(75)-C(40)	120(2)	O(27)-W(6)-O(9)	72.3(4)
C(33)-C(76)-C(77)	117(2)	O(15)-W(6)-O(9)	83.2(4)
C(78)-C(77)-F(4)	118(2)	O(60)-W(7)-O(48)	102.8(5)
C(78)-C(77)-C(76)	124(2)	O(60)-W(7)-O(54)	97.4(5)
F(4)-C(77)-C(76)	118(2)	O(48)-W(7)-O(54)	86.2(5)
C(77)-C(78)-C(66)	116(2)	O(60)-W(7)-O(40)	99.2(5)
F(5)-C(79)-C(75)	121(2)	O(48)-W(7)-O(40)	157.9(4)
F(5)-C(79)-C(81)	115(2)	O(54)-W(7)-O(40)	89.5(5)
C(75)-C(79)-C(81)	124(3)	O(60)-W(7)-O(35)	97.5(5)
C(42)-C(80)-C(75)	123(3)	O(48)-W(7)-O(35)	88.3(4)
C(82)-C(81)-C(79)	116(3)	O(54)-W(7)-O(35)	165.0(4)
C(81)-C(82)-F(7)	120(3)	O(40)-W(7)-O(35)	90.4(4)
C(81)-C(82)-C(42)	127(3)	O(60)-W(7)-O(59)	172.2(5)
F(7)-C(82)-C(42)	113(3)	O(48)-W(7)-O(59)	84.9(4)

F(1)-C(83)-C(84)	120.5(19)	O(54)-W(7)-O(59)	82.2(4)
F(1)-C(83)-C(25)	116(2)	O(40)-W(7)-O(59)	73.1(4)
C(84)-C(83)-C(25)	124(2)	O(35)-W(7)-O(59)	83.4(4)
C(83)-C(84)-C(85)	118.6(18)	O(21)-W(8)-O(12)	102.8(5)
C(83)-C(84)-C(45)	121.6(19)	O(21)-W(8)-O(35)	97.2(5)
C(85)-C(84)-C(45)	119.7(16)	O(12)-W(8)-O(35)	89.8(4)
C(84)-C(85)-C(26)	120(2)	O(21)-W(8)-O(0AA)	98.5(5)
C(49)-N(1)-N(29)	102.6(15)	O(12)-W(8)-O(0AA)	158.7(4)
C(49)-N(1)-Cu(1)	120.8(11)	O(35)-W(8)-O(0AA)	88.8(5)
N(29)-N(1)-Cu(1)	136.2(14)	O(21)-W(8)-O(1AA)	97.5(5)
C(2)-N(2)-N(8)	104.4(17)	O(12)-W(8)-O(1AA)	87.2(5)
C(62)-N(3)-C(61)	103.5(16)	O(35)-W(8)-O(1AA)	165.3(4)
C(62)-N(3)-Cu(1)	130.8(13)	O(0AA)-W(8)-O(1AA)	88.8(5)
C(61)-N(3)-Cu(1)	125.6(13)	O(21)-W(8)-O(5)	172.2(5)
C(3)-N(4)-N(28)	101.4(19)	O(12)-W(8)-O(5)	84.8(4)
C(18)-N(5)-N(35)	110.2(14)	O(35)-W(8)-O(5)	84.8(4)
C(18)-N(5)-C(21)	129.0(15)	O(0AA)-W(8)-O(5)	73.9(4)
N(35)-N(5)-C(21)	120.5(14)	O(1AA)-W(8)-O(5)	80.6(4)
C(18)-N(6)-C(19)	103.5(15)	O(44)-W(9)-O(43)	100.1(5)
C(18)-N(6)-Cu(2)	119.8(12)	O(44)-W(9)-O(45)	103.3(5)
C(19)-N(6)-Cu(2)	136.5(13)	O(43)-W(9)-O(45)	87.9(4)
C(1)-N(7)-C(2)	104.8(16)	O(44)-W(9)-O(42)	99.0(5)
C(1)-N(7)-Cu(2)	127.7(13)	O(43)-W(9)-O(42)	92.7(4)
C(2)-N(7)-Cu(2)	127.4(13)	O(45)-W(9)-O(42)	157.2(4)
C(1)-N(8)-N(2)	109.6(16)	O(44)-W(9)-O(31)	95.9(5)
C(1)-N(8)-C(10)	129.8(18)	O(43)-W(9)-O(31)	163.9(5)
N(2)-N(8)-C(10)	120.5(17)	O(45)-W(9)-O(31)	86.7(4)
C(6)-N(9)-C(44)	103.1(15)	O(42)-W(9)-O(31)	86.6(4)
C(6)-N(9)-Cu(2)	126.9(12)	O(44)-W(9)-O(36)	171.9(5)
C(44)-N(9)-Cu(2)	130.0(12)	O(43)-W(9)-O(36)	83.5(4)
C(6)-N(10)-N(40)	107.7(16)	O(45)-W(9)-O(36)	84.0(4)
C(6)-N(10)-C(8)	130.9(19)	O(42)-W(9)-O(36)	73.4(4)
N(40)-N(10)-C(8)	121.3(18)	O(31)-W(9)-O(36)	80.8(4)
C(28)-N(11)-N(23)	105.2(17)	O(14)-W(10)-O(8)	101.7(5)
C(28)-N(11)-Cu(4)	132.6(14)	O(14)-W(10)-O(15)	98.1(5)
N(23)-N(11)-Cu(4)	122.2(13)	O(8)-W(10)-O(15)	87.8(4)
Cu(4)-O(102)-Cu(5)	99.5(5)	O(14)-W(10)-O(0AA)	102.2(5)
C(4)-N(14)-C(43)	104.1(15)	O(8)-W(10)-O(0AA)	155.9(5)

C(4)-N(14)-Cu(2)	127.6(12)	O(15)-W(10)-O(0AA)	92.3(5)
C(43)-N(14)-Cu(2)	128.2(13)	O(14)-W(10)-O(30)	96.6(5)
C(43)-N(15)-N(22)	104.5(16)	O(8)-W(10)-O(30)	86.3(4)
C(32)-O(16)-Cu(4)	129.0(12)	O(15)-W(10)-O(30)	165.0(4)
C(32)-O(16)-Cu(5)	129.1(11)	O(0AA)-W(10)-O(30)	87.5(4)
Cu(4)-O(16)-Cu(5)	101.2(5)	O(14)-W(10)-O(5)	175.2(5)
C(60)-N(17)-C(57)	103.9(16)	O(8)-W(10)-O(5)	83.0(4)
C(60)-N(17)-Cu(3)	126.8(13)	O(15)-W(10)-O(5)	82.8(4)
C(57)-N(17)-Cu(3)	129.2(13)	O(0AA)-W(10)-O(5)	73.1(4)
C(117)-N(18)-C(55)	104.2(17)	O(30)-W(10)-O(5)	82.7(4)
C(117)-N(18)-Cu(3)	128.3(14)	O(4)-W(11)-O(41)	104.2(5)
C(55)-N(18)-Cu(3)	126.8(13)	O(4)-W(11)-O(42)	98.1(5)
C(52)-N(19)-C(3)	103.8(17)	O(41)-W(11)-O(42)	157.7(4)
C(52)-N(19)-Cu(3)	127.0(14)	O(4)-W(11)-O(46)	98.5(5)
C(3)-N(19)-Cu(3)	122.2(15)	O(41)-W(11)-O(46)	87.1(5)
C(119)-N(20)-C(121)	106(2)	O(42)-W(11)-O(46)	90.4(5)
C(119)-N(20)-Cu(3)	128.7(17)	O(4)-W(11)-O(32)	97.0(5)
C(121)-N(20)-Cu(3)	124.7(15)	O(41)-W(11)-O(32)	87.7(4)
C(49)-N(21)-C(12)	111.7(14)	O(42)-W(11)-O(32)	88.9(4)
C(49)-N(21)-C(11)	126.7(14)	O(46)-W(11)-O(32)	164.4(4)
C(12)-N(21)-C(11)	121.3(15)	O(4)-W(11)-O(36)	171.9(5)
C(4)-N(22)-N(15)	108.4(16)	O(41)-W(11)-O(36)	83.9(4)
C(4)-N(22)-C(39)	128.2(17)	O(42)-W(11)-O(36)	73.8(4)
N(15)-N(22)-C(39)	123.2(16)	O(46)-W(11)-O(36)	82.0(4)
C(47)-N(23)-N(11)	109.9(17)	O(32)-W(11)-O(36)	82.9(4)
C(47)-N(23)-C(31)	127.8(17)	O(26)-W(12)-O(19)	102.6(5)
N(11)-N(23)-C(31)	121.8(16)	O(26)-W(12)-O(28)	101.7(5)
C(28)-N(24)-C(47)	104.9(19)	O(19)-W(12)-O(28)	155.7(4)
C(5)-N(25)-N(26)	112(2)	O(26)-W(12)-O(18)	102.8(5)
C(5)-N(25)-C(48)	129(2)	O(19)-W(12)-O(18)	84.7(5)
N(26)-N(25)-C(48)	119.8(17)	O(28)-W(12)-O(18)	88.8(5)
C(46)-N(26)-N(25)	104(2)	O(26)-W(12)-O(25)	101.0(5)
C(46)-N(26)-Cu(5)	132(2)	O(19)-W(12)-O(25)	89.2(5)
N(25)-N(26)-Cu(5)	122.5(14)	O(28)-W(12)-O(25)	87.4(5)
C(55)-N(27)-N(39)	110.4(17)	O(18)-W(12)-O(25)	156.1(4)
C(55)-N(27)-C(41)	129.2(17)	O(26)-W(12)-O(9)	171.7(5)
N(39)-N(27)-C(41)	119.4(17)	O(19)-W(12)-O(9)	83.5(4)
C(52)-N(28)-N(4)	112.1(18)	O(28)-W(12)-O(9)	72.4(4)

C(52)-N(28)-C(53)	128.2(18)	O(18)-W(12)-O(9)	83.2(4)
N(4)-N(28)-C(53)	119.3(19)	O(25)-W(12)-O(9)	73.2(4)
C(12)-N(29)-N(1)	114.4(18)	O(7)-W(13)-O(33)	98.9(5)
C(62)-N(30)-N(36)	109.5(15)	O(7)-W(13)-O(41)	102.7(5)
C(62)-N(30)-C(118)	133.6(17)	O(33)-W(13)-O(41)	88.5(5)
N(36)-N(30)-C(118)	116.8(16)	O(7)-W(13)-O(56)	99.3(5)
C(5)-N(31)-C(46)	106(3)	O(33)-W(13)-O(56)	90.4(4)
N(18)-C(117)-N(39)	113(2)	O(41)-W(13)-O(56)	157.8(5)
C(19)-N(35)-N(5)	103.2(14)	O(7)-W(13)-O(62)	97.3(5)
C(61)-N(36)-N(30)	102.9(16)	O(33)-W(13)-O(62)	163.6(4)
W(5)-O(2)-W(2)	150.9(6)	O(41)-W(13)-O(62)	85.4(5)
P(1)-O(3)-W(5)	128.1(6)	O(56)-W(13)-O(62)	89.6(4)
P(1)-O(3)-W(17)	127.4(6)	O(7)-W(13)-O(38)	171.7(5)
W(5)-O(3)-W(17)	90.3(4)	O(33)-W(13)-O(38)	82.7(4)
P(1)-O(5)-W(8)	127.9(6)	O(41)-W(13)-O(38)	85.4(4)
P(1)-O(5)-W(10)	127.7(6)	O(56)-W(13)-O(38)	72.5(4)
W(8)-O(5)-W(10)	90.7(4)	O(62)-W(13)-O(38)	81.6(4)
P(1)-O(6)-W(3)	128.3(6)	O(55)-W(14)-O(62)	103.2(5)
P(1)-O(6)-W(2)	127.9(6)	O(55)-W(14)-O(46)	103.9(5)
W(3)-O(6)-W(2)	91.2(3)	O(62)-W(14)-O(46)	86.8(5)
W(10)-O(8)-W(3)	150.9(6)	O(55)-W(14)-O(50)	98.7(5)
P(1)-O(9)-W(16)	124.1(6)	O(62)-W(14)-O(50)	89.0(5)
P(1)-O(9)-W(6)	126.0(6)	O(46)-W(14)-O(50)	157.3(4)
W(16)-O(9)-W(6)	91.2(3)	O(55)-W(14)-O(49)	99.9(5)
P(1)-O(9)-W(12)	124.8(6)	O(62)-W(14)-O(49)	156.8(4)
W(16)-O(9)-W(12)	90.6(3)	O(46)-W(14)-O(49)	88.8(5)
W(6)-O(9)-W(12)	89.4(3)	O(50)-W(14)-O(49)	86.3(5)
W(5)-O(10)-W(17)	121.5(5)	O(55)-W(14)-O(37)	168.8(4)
W(8)-O(12)-W(17)	152.3(6)	O(62)-W(14)-O(37)	83.8(4)
W(8)-O(0AA)-W(10)	122.3(5)	O(46)-W(14)-O(37)	85.0(4)
W(10)-O(15)-W(6)	150.9(6)	O(50)-W(14)-O(37)	72.4(4)
W(16)-O(1AA)-W(8)	149.3(6)	O(49)-W(14)-O(37)	73.2(4)
W(16)-O(17)-W(17)	150.6(7)	O(51)-W(15)-O(52)	100.0(6)
W(5)-O(18)-W(12)	152.2(6)	O(51)-W(15)-O(47)	102.6(5)
W(12)-O(19)-W(2)	151.9(6)	O(52)-W(15)-O(47)	90.6(5)
W(2)-O(20)-W(3)	121.7(5)	O(51)-W(15)-O(43)	101.8(6)
W(3)-O(22)-Cu(2)	157.8(7)	O(52)-W(15)-O(43)	158.2(5)
W(6)-O(23)-W(3)	152.5(6)	O(47)-W(15)-O(43)	85.6(4)

W(6)-O(25)-W(12)	122.9(5)	O(51)-W(15)-O(49)	101.4(5)
W(6)-O(27)-W(16)	123.0(6)	O(52)-W(15)-O(49)	87.4(5)
W(12)-O(28)-W(16)	122.7(6)	O(47)-W(15)-O(49)	155.9(5)
W(1)-O(30)-W(10)	161.5(6)	O(43)-W(15)-O(49)	87.4(4)
W(3)-O(31)-W(9)	163.1(6)	O(51)-W(15)-O(37)	171.6(5)
W(2)-O(32)-W(11)	163.4(6)	O(52)-W(15)-O(37)	74.2(4)
W(13)-O(33)-W(5)	163.4(6)	O(47)-W(15)-O(37)	83.7(4)
W(17)-O(34)-W(4)	163.8(7)	O(43)-W(15)-O(37)	84.1(4)
W(8)-O(35)-W(7)	161.1(6)	O(49)-W(15)-O(37)	72.7(4)
P(2)-O(36)-W(9)	126.7(6)	O(66)#5-W(16)-O(1AA)	103.1(5)
P(2)-O(36)-W(11)	128.9(6)	O(66)#5-W(16)-O(17)	101.1(5)
W(9)-O(36)-W(11)	90.1(3)	O(1AA)-W(16)-O(17)	87.7(5)
P(2)-O(37)-W(14)	125.4(6)	O(66)#5-W(16)-O(27)	100.5(5)
P(2)-O(37)-W(15)	124.9(6)	O(1AA)-W(16)-O(27)	89.3(5)
W(14)-O(37)-W(15)	90.8(3)	O(17)-W(16)-O(27)	158.3(4)
P(2)-O(37)-W(18)	124.4(5)	O(66)#5-W(16)-O(28)	98.6(5)
W(14)-O(37)-W(18)	90.9(3)	O(1AA)-W(16)-O(28)	158.3(4)
W(15)-O(37)-W(18)	89.7(3)	O(17)-W(16)-O(28)	89.0(5)
P(2)-O(38)-W(13)	128.0(6)	O(27)-W(16)-O(28)	85.9(5)
P(2)-O(38)-W(4)	127.5(6)	O(66)#5-W(16)-O(9)	170.7(5)
W(13)-O(38)-W(4)	91.3(4)	O(1AA)-W(16)-O(9)	84.1(4)
W(7)-O(40)-W(1)	121.4(5)	O(17)-W(16)-O(9)	84.9(4)
W(13)-O(41)-W(11)	151.2(6)	O(27)-W(16)-O(9)	73.5(4)
W(11)-O(42)-W(9)	122.7(5)	O(28)-W(16)-O(9)	74.2(4)
W(9)-O(43)-W(15)	149.7(6)	O(11)-W(17)-O(12)	102.7(5)
W(1)-O(45)-W(9)	151.1(6)	O(11)-W(17)-O(34)	100.6(5)
W(14)-O(46)-W(11)	149.4(6)	O(12)-W(17)-O(34)	87.3(5)
W(15)-O(47)-W(1)	152.2(6)	O(11)-W(17)-O(10)	99.9(5)
W(7)-O(48)-W(4)	153.1(6)	O(12)-W(17)-O(10)	157.3(4)
W(15)-O(49)-W(14)	123.3(6)	O(34)-W(17)-O(10)	90.8(5)
W(18)-O(50)-W(14)	125.1(5)	O(11)-W(17)-O(17)	97.0(5)
W(15)-O(52)-W(18)	122.8(6)	O(12)-W(17)-O(17)	86.0(5)
W(18)-O(54)-W(7)	150.5(6)	O(34)-W(17)-O(17)	162.1(4)
W(13)-O(56)-W(4)	124.2(6)	O(10)-W(17)-O(17)	89.1(5)
W(18)-O(57)-W(4)	149.0(6)	O(11)-W(17)-O(3)	172.9(5)
P(2)-O(59)-W(1)	129.1(6)	O(12)-W(17)-O(3)	83.8(4)
P(2)-O(59)-W(7)	126.6(6)	O(34)-W(17)-O(3)	82.4(4)
W(1)-O(59)-W(7)	91.7(4)	O(10)-W(17)-O(3)	73.5(4)

W(14)-O(62)-W(13)	151.5(6)	O(17)-W(17)-O(3)	80.5(4)
W(16)#3-O(66)-Cu(3)	145.2(7)	O(53)-W(18)-O(57)	101.2(6)
O(5)-P(1)-O(3)	112.7(6)	O(53)-W(18)-O(54)	103.3(5)
O(5)-P(1)-O(6)	112.1(6)	O(57)-W(18)-O(54)	87.1(5)
O(3)-P(1)-O(6)	111.5(6)	O(53)-W(18)-O(50)	101.5(5)
O(5)-P(1)-O(9)	106.4(6)	O(57)-W(18)-O(50)	89.0(5)
O(3)-P(1)-O(9)	107.7(6)	O(54)-W(18)-O(50)	155.2(4)
O(6)-P(1)-O(9)	106.0(5)	O(53)-W(18)-O(52)	100.7(6)
O(36)-P(2)-O(38)	111.4(6)	O(57)-W(18)-O(52)	158.1(4)
O(36)-P(2)-O(59)	112.2(6)	O(54)-W(18)-O(52)	88.7(5)
O(38)-P(2)-O(59)	113.1(6)	O(50)-W(18)-O(52)	85.8(5)
O(36)-P(2)-O(37)	106.3(6)	O(53)-W(18)-O(37)	170.9(5)
O(38)-P(2)-O(37)	106.4(6)	O(57)-W(18)-O(37)	84.8(4)
O(59)-P(2)-O(37)	106.9(5)	O(54)-W(18)-O(37)	83.7(4)
N(3)-Cu(1)-N(3)#4	180.0	O(50)-W(18)-O(37)	71.5(4)
N(3)-Cu(1)-N(1)#4	90.0(6)	O(52)-W(18)-O(37)	73.3(4)
N(3)#4-Cu(1)-N(1)#4	90.0(6)	C(103)-C(101)-C(106)	120.0
N(3)-Cu(1)-N(1)	90.0(6)	C(101)-C(103)-C(105)	120.0
N(3)#4-Cu(1)-N(1)	90.0(6)	F(8)-C(105)-C(102)	112(3)
N(1)#4-Cu(1)-N(1)	180.0	F(8)-C(105)-C(103)	128(3)
N(9)-Cu(2)-N(14)	89.0(6)	C(102)-C(105)-C(103)	120.0
N(9)-Cu(2)-N(6)	88.1(6)	C(105)-C(102)-C(104)	120.0
N(14)-Cu(2)-N(6)	177.0(6)	C(106)-C(104)-C(102)	120.0
N(9)-Cu(2)-N(7)	175.9(6)	C(106)-C(104)-F(9)	115(2)
N(14)-Cu(2)-N(7)	92.3(6)	C(102)-C(104)-F(9)	125(2)
N(6)-Cu(2)-N(7)	90.6(6)	C(104)-C(106)-C(101)	120.0
N(9)-Cu(2)-O(103)	91.7(7)	C(104)-C(106)-C(74)	120.1(19)
N(14)-Cu(2)-O(103)	84.7(8)	C(101)-C(106)-C(74)	119.6(19)
N(6)-Cu(2)-O(103)	96.2(8)	O(100)-C(7)-C(111)	107(2)
N(7)-Cu(2)-O(103)	84.5(8)	O(100)-C(7)-C(118)	112.2(17)
N(9)-Cu(2)-O(22)	98.8(5)	C(111)-C(7)-C(118)	109.3(18)
N(14)-Cu(2)-O(22)	92.3(5)	O(100)-C(7)-C(120)	105.2(19)
N(6)-Cu(2)-O(22)	87.3(5)	C(111)-C(7)-C(120)	118(2)
N(7)-Cu(2)-O(22)	85.0(5)	C(118)-C(7)-C(120)	105.0(19)
O(103)-Cu(2)-O(22)	169.0(7)	N(30)-C(118)-C(7)	109.7(17)
N(17)-Cu(3)-N(20)	93.3(7)	N(101)-N(100)-C(119)	105(3)
N(17)-Cu(3)-N(19)	91.9(7)	N(20)-C(119)-N(100)	110(3)
N(20)-Cu(3)-N(19)	171.0(6)	N(101)#6-C(120)-C(7)	108(2)

N(17)-Cu(3)-N(18)	177.4(6)	N(101)-C(121)-N(20)	103(2)
N(20)-Cu(3)-N(18)	88.6(7)	N(100)-N(101)-C(121)	115(3)
N(19)-Cu(3)-N(18)	86.4(7)	N(100)-N(101)-C(120)#7	121(3)
N(17)-Cu(3)-O(66)	88.7(5)	C(121)-N(101)-C(120)#7	124(2)
N(20)-Cu(3)-O(66)	85.9(6)	C(116)-C(111)-C(114)	120.0
N(19)-Cu(3)-O(66)	101.5(5)	C(116)-C(111)-C(7)	110(2)
N(18)-Cu(3)-O(66)	89.7(5)	C(114)-C(111)-C(7)	130(2)
O(16)-Cu(4)-O(102)	80.9(5)	C(111)-C(116)-C(115)	120.0
O(16)-Cu(4)-N(11)	92.8(6)	C(111)-C(116)-F(12)	131(3)
O(102)-Cu(4)-N(11)	173.6(6)	C(115)-C(116)-F(12)	109(3)
O(16)-Cu(4)-O(58)	172.9(6)	C(113)-C(115)-C(116)	120.0
O(102)-Cu(4)-O(58)	93.1(5)	F(11)-C(113)-C(112)	125(2)
N(11)-Cu(4)-O(58)	93.3(6)	F(11)-C(113)-C(115)	115(2)
O(16)-Cu(4)-Cu(5)	39.9(3)	C(112)-C(113)-C(115)	120.0
O(102)-Cu(4)-Cu(5)	41.0(4)	C(113)-C(112)-C(114)	120.0
N(11)-Cu(4)-Cu(5)	132.7(5)	C(112)-C(114)-C(111)	120.0
O(58)-Cu(4)-Cu(5)	133.9(4)	F(13B)-F(13A)-C(17)	64(3)
O(16)-Cu(5)-N(26)	91.4(7)	F(13A)-F(13B)-C(17)	62(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y-1/2,-z+1/2; #2-x+1/2,y+1/2,-z+1/2;#3 x-1,y,z; #4 -x+2,-y+2,-z; #5 x+1,y,z; #6-x+3/2,y+1/2,-z+1/2;#7 -x+3/2,y-1/2,-z+1/2