Supplementary Information

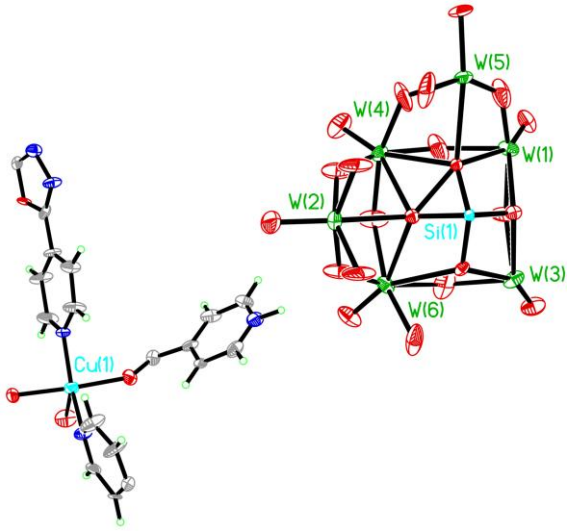

Fig. S1 ORTEP drawing of compound **1** with thermal ellipsoids at 30% probability. Color code: W (green), Cu (lightblue), Si (cyan), O (red) and N (blue).

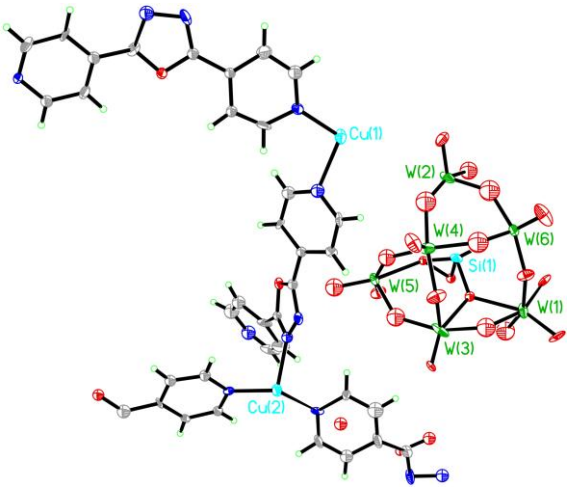

Fig. S2 ORTEP drawing of compound **2** with thermal ellipsoids at 30% probability. Colour code: W (green), Cu (lightblue), Si (cyan), O (red) and N (blue).

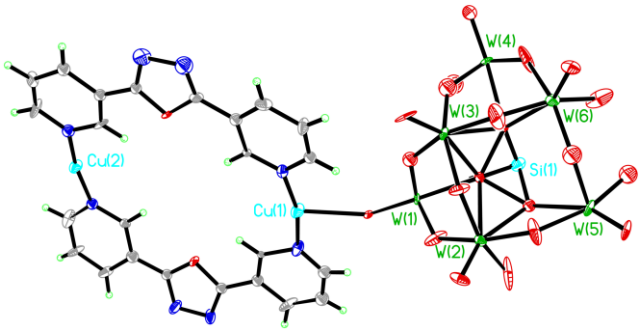

Fig. S3 ORTEP drawing of compound **3** with thermal ellipsoids at 30% probability. Colour code: W (green), Cu (lightblue), Si (cyan), O (red) and N (blue).

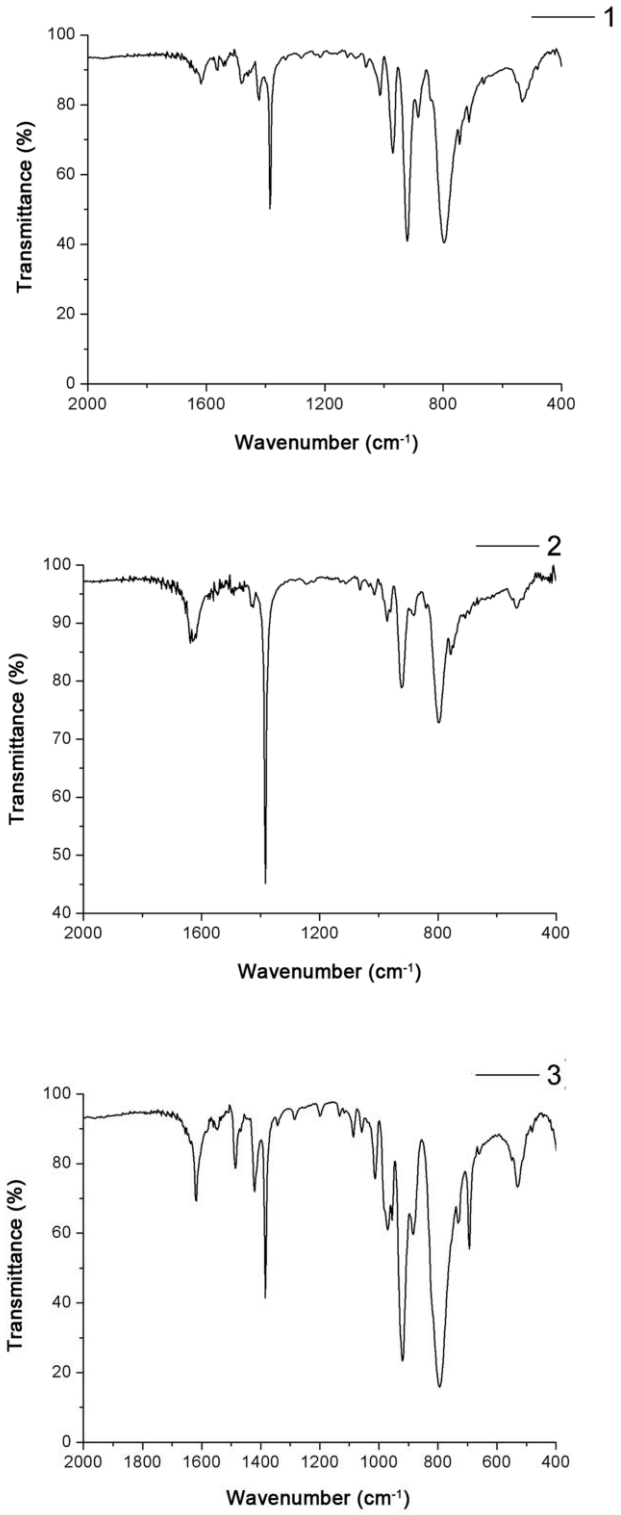

Fig. S4 IR spectra of **1, 2** and **3**

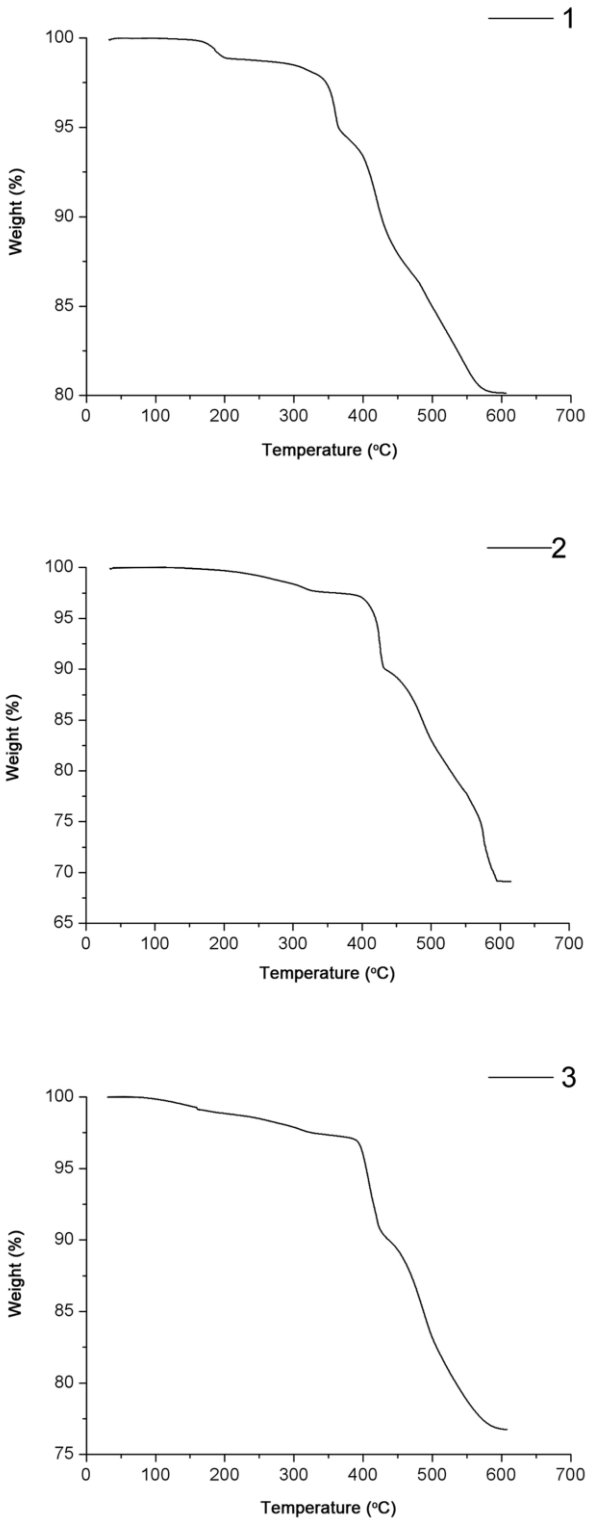

Fig. S5 TG curves of **1, 2** and **3**

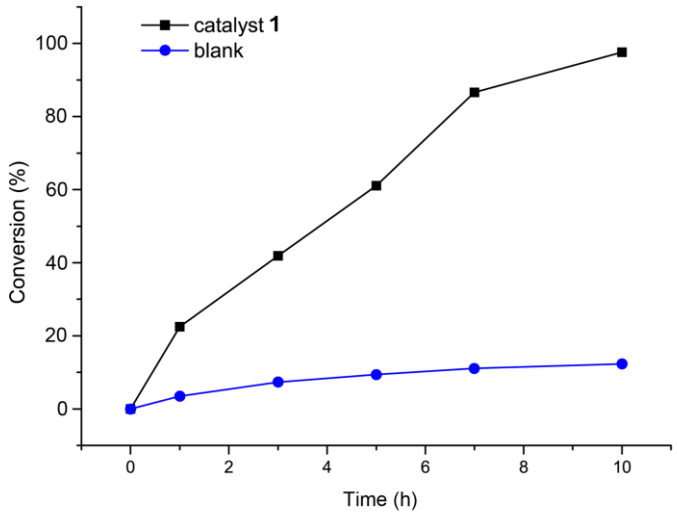

Fig. S6 The conversion of styene using TBHP as oxidant with/without catalyst **1**.

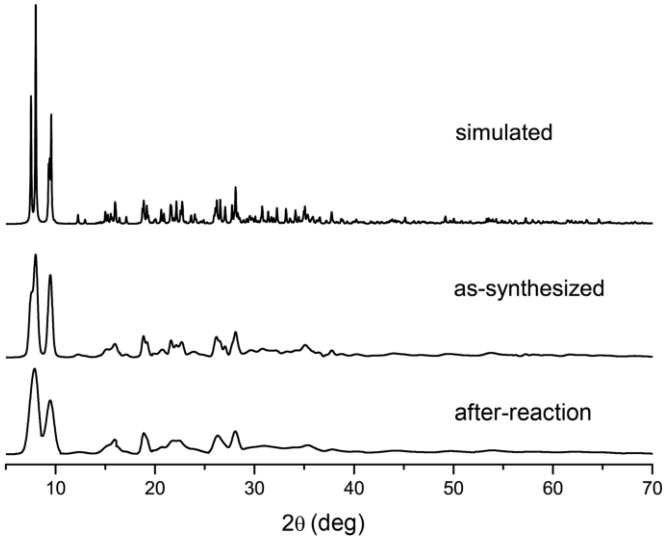

Fig. S7 Powder XRD patterns of simulated, as-synthesized and after-reaction compound **1**.

Table S1 The selected bond lengths (Å) for **1**

Si(1)-O(23)	1.569(18)	W(4)-O(13)	1.870(12)	O(24)-Cu(1)	2.012(12)
Si(1)-O(23)#1	1.569(18)	W(4)-O(10)	1.880(9)	O(25)-C(18)#2	1.194(17)
Si(1)-O(21)#1	1.652(18)	W(4)-O(14)	1.898(11)	O(25)-Cu(1)	2.113(10)
Si(1)-O(21)	1.652(18)	W(4)-O(20)	2.328(16)	O(26)-Cu(1)	2.032(10)
Si(1)-O(20)#1	1.674(15)	W(4)-O(23)	2.432(16)	C(1)-N(1)	1.316(16)
Si(1)-O(20)	1.674(15)	W(5)-O(3)	1.700(8)	C(1)-C(2)	1.412(18)
Si(1)-O(22)#1	1.701(16)	W(5)-O(11)	1.845(12)	C(2)-C(3)	1.371(17)
Si(1)-O(22)	1.701(16)	W(5)-O(18)#1	1.873(12)	C(3)-C(4)	1.330(18)
W(1)-O(6)	1.613(10)	W(5)-O(17)	1.877(12)	C(3)-C(12)#3	1.438(18)
W(1)-O(1)	1.892(9)	W(5)-O(14)	1.882(12)	C(4)-C(5)	1.389(19)
W(1)-O(17)	1.898(10)	W(5)-O(22)#1	2.370(15)	C(5)-N(1)	1.277(17)
W(1)-O(13)	1.902(13)	W(5)-O(20)	2.406(15)	C(6)-N(2)	1.311(18)
W(1)-O(7)#1	1.910(11)	W(6)-O(4)	1.657(9)	C(6)-C(7)	1.433(19)
W(1)-O(20)	2.385(17)	W(6)-O(16)	1.877(12)	C(7)-C(8)	1.353(19)
W(1)-O(21)	2.409(17)	W(6)-O(12)	1.883(11)	C(8)-C(9)	1.327(18)
W(2)-O(15)	1.636(12)	W(6)-O(18)	1.919(10)	C(8)-C(11)	1.438(17)
W(2)-O(5)	1.883(9)	W(6)-O(10)	1.925(10)	C(9)-C(10)	1.407(19)
W(2)-O(7)	1.888(10)	W(6)-O(22)	2.322(18)	C(10)-N(2)	1.310(17)
W(2)-O(9)	1.910(10)	W(6)-O(23)	2.456(16)	C(11)-N(3)	1.295(16)
W(2)-O(12)	1.925(9)	O(5)-W(3)#1	1.884(11)	C(12)-N(4)	1.285(16)
W(2)-O(21)#1	2.277(18)	O(7)-W(1)#1	1.910(11)	C(12)-C(3)#4	1.438(18)
W(2)-O(23)	2.363(19)	O(11)-W(3)#1	1.914(10)	C(13)-N(5)	1.282(19)
W(3)-O(8)	1.647(9)	O(18)-W(5)#1	1.873(12)	C(13)-C(14)	1.45(2)
W(3)-O(16)	1.881(13)	O(19)-C(11)	1.350(14)	C(14)-C(15)	1.35(2)
W(3)-O(5)#1	1.884(11)	O(19)-C(12)	1.366(14)	C(15)-C(16)	1.344(18)
W(3)-O(1)	1.893(10)	O(20)-O(23)	1.82(2)	C(15)-C(18)	1.54(2)
W(3)-O(11)#1	1.914(10)	O(21)-O(23)#1	1.74(2)	C(17)-N(5)	1.32(2)
W(3)-O(22)	2.361(17)	O(21)-W(2)#1	2.277(18)	C(18)-O(25)#2	1.194(17)
W(3)-O(21)	2.444(15)	O(22)-W(5)#1	2.370(15)	Cu(1)-N(2)	1.967(12)
W(4)-O(2)	1.680(9)	O(23)-O(21)#1	1.74(2)	Cu(1)-N(1)	1.992(11)
W(4)-O(9)	1.867(12)	O(24)-C(18)	1.292(19)	N(3)-N(4)	1.404(14)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z #2 -x+1,-y+1,-z+2 #3 x,y+1,z #4 x,y-1,z

Table S2 The selected bond angles (º) for **1**

O(23)-Si(1)-O(23)#1	180.0(10)	Si(1)-O(21)-W(1)	119.8(9)
O(23)-Si(1)-O(21)#1	65.3(8)	O(23)#1-O(21)-W(1)	135.1(10)
O(23)#1-Si(1)-O(21)#1	114.7(8)	W(2)#1-O(21)-W(1)	97.4(7)
O(23)-Si(1)-O(21)	114.7(8)	Si(1)-O(21)-W(3)	117.8(9)
O(23)#1-Si(1)-O(21)	65.3(8)	O(23)#1-O(21)-W(3)	130.0(10)
O(21)#1-Si(1)-O(21)	180.0(15)	W(2)#1-O(21)-W(3)	95.8(6)
O(23)-Si(1)-O(20)#1	111.9(8)	W(1)-O(21)-W(3)	93.4(5)
O(23)#1-Si(1)-O(20)#1	68.1(8)	Si(1)-O(22)-W(6)	120.6(8)
O(21)#1-Si(1)-O(20)#1	72.0(8)	Si(1)-O(22)-W(3)	119.9(10)
O(21)-Si(1)-O(20)#1	108.0(8)	W(6)-O(22)-W(3)	97.5(6)

O(23)-Si(1)-O(20)	68.1(8)	Si(1)-O(22)-W(5)#1	119.3(7)
O(23)#1-Si(1)-O(20)	111.9(8)	W(6)-O(22)-W(5)#1	97.7(7)
O(21)#1-Si(1)-O(20)	108.0(8)	W(3)-O(22)-W(5)#1	96.8(6)
O(21)-Si(1)-O(20)	72.0(8)	Si(1)-O(23)-O(21)#1	59.6(8)
O(20)#1-Si(1)-O(20)	180.0(10)	Si(1)-O(23)-O(20)	58.7(8)
O(23)-Si(1)-O(22)#1	107.8(8)	O(21)#1-O(23)-O(20)	98.2(11)
O(23)#1-Si(1)-O(22)#1	72.2(8)	Si(1)-O(23)-W(2)	125.0(8)
O(21)#1-Si(1)-O(22)#1	73.1(8)	O(21)#1-O(23)-W(2)	65.4(8)
O(21)-Si(1)-O(22)#1	106.9(8)	O(20)-O(23)-W(2)	133.2(9)
O(20)#1-Si(1)-O(22)#1	107.4(7)	Si(1)-O(23)-W(4)	123.2(10)
O(20)-Si(1)-O(22)#1	72.6(7)	O(21)#1-O(23)-W(4)	133.9(10)
O(23)-Si(1)-O(22)	72.2(8)	O(20)-O(23)-W(4)	64.6(7)
O(23)#1-Si(1)-O(22)	107.8(8)	W(2)-O(23)-W(4)	94.8(6)
O(21)#1-Si(1)-O(22)	106.9(8)	Si(1)-O(23)-W(6)	119.6(8)
O(21)-Si(1)-O(22)	73.1(8)	O(21)#1-O(23)-W(6)	128.4(10)
O(20)#1-Si(1)-O(22)	72.6(7)	O(20)-O(23)-W(6)	126.5(9)
O(20)-Si(1)-O(22)	107.4(7)	W(2)-O(23)-W(6)	93.9(7)
O(22)#1-Si(1)-O(22)	180.0(10)	W(4)-O(23)-W(6)	92.1(5)
O(6)-W(1)-O(1)	100.7(5)	C(18)-O(24)-Cu(1)	133.0(11)
O(6)-W(1)-O(17)	102.5(5)	C(18)#2-O(25)-Cu(1)	134.8(11)
O(1)-W(1)-O(17)	156.8(6)	N(1)-C(1)-C(2)	122.0(14)
O(6)-W(1)-O(13)	102.9(6)	C(3)-C(2)-C(1)	116.6(13)
O(1)-W(1)-O(13)	86.7(5)	C(4)-C(3)-C(2)	120.0(14)
O(17)-W(1)-O(13)	87.1(5)	C(4)-C(3)-C(12)#3	120.1(14)
O(6)-W(1)-O(7)#1	99.5(6)	C(2)-C(3)-C(12)#3	119.7(13)
O(1)-W(1)-O(7)#1	90.2(4)	C(3)-C(4)-C(5)	118.5(14)
O(17)-W(1)-O(7)#1	87.1(5)	N(1)-C(5)-C(4)	123.3(15)
O(13)-W(1)-O(7)#1	157.6(6)	N(2)-C(6)-C(7)	120.5(16)
O(6)-W(1)-O(20)	157.7(5)	C(8)-C(7)-C(6)	120.3(15)
O(1)-W(1)-O(20)	93.9(6)	C(9)-C(8)-C(7)	117.8(13)
O(17)-W(1)-O(20)	63.6(5)	C(9)-C(8)-C(11)	121.3(14)
O(13)-W(1)-O(20)	61.1(5)	C(7)-C(8)-C(11)	120.9(14)
O(7)#1-W(1)-O(20)	97.1(6)	C(8)-C(9)-C(10)	120.0(16)
O(6)-W(1)-O(21)	154.1(6)	N(2)-C(10)-C(9)	122.9(16)
O(1)-W(1)-O(21)	64.5(5)	N(3)-C(11)-O(19)	111.9(12)
O(17)-W(1)-O(21)	94.2(6)	N(3)-C(11)-C(8)	130.1(13)
O(13)-W(1)-O(21)	97.5(6)	O(19)-C(11)-C(8)	117.7(13)
O(7)#1-W(1)-O(21)	61.4(6)	N(4)-C(12)-O(19)	110.6(12)
O(20)-W(1)-O(21)	48.1(5)	N(4)-C(12)-C(3)#4	128.4(14)
O(15)-W(2)-O(5)	101.0(6)	O(19)-C(12)-C(3)#4	120.9(12)
O(15)-W(2)-O(7)	101.0(6)	N(5)-C(13)-C(14)	119.4(17)
O(5)-W(2)-O(7)	90.6(4)	C(15)-C(14)-C(13)	117.9(17)
O(15)-W(2)-O(9)	99.6(5)	C(16)-C(15)-C(14)	121.0(17)
O(5)-W(2)-O(9)	88.1(4)	C(16)-C(15)-C(18)	121.1(17)
O(7)-W(2)-O(9)	159.2(6)	C(14)-C(15)-C(18)	117.8(15)

O(15)-W(2)-O(12)	99.3(6)	C(15)-C(16)-C(17)	118.6(17)
O(5)-W(2)-O(12)	159.6(6)	N(5)-C(17)-C(16)	119.5(16)
O(7)-W(2)-O(12)	87.5(4)	O(25)#2-C(18)-O(24)	125.6(18)
O(9)-W(2)-O(12)	86.4(4)	O(25)#2-C(18)-C(15)	123.8(18)
O(15)-W(2)-O(21)#1	158.5(6)	O(24)-C(18)-C(15)	110.6(15)
O(5)-W(2)-O(21)#1	65.1(5)	N(2)-Cu(1)-N(1)	152.3(6)
O(7)-W(2)-O(21)#1	64.5(6)	N(2)-Cu(1)-O(24)	89.4(5)
O(9)-W(2)-O(21)#1	96.3(6)	N(1)-Cu(1)-O(24)	84.1(5)
O(12)-W(2)-O(21)#1	96.0(6)	N(2)-Cu(1)-O(26)	90.1(5)
O(15)-W(2)-O(23)	157.5(6)	N(1)-Cu(1)-O(26)	89.9(5)
O(5)-W(2)-O(23)	93.8(6)	O(24)-Cu(1)-O(26)	165.9(4)
O(7)-W(2)-O(23)	95.6(6)	N(2)-Cu(1)-O(25)	108.4(5)
O(9)-W(2)-O(23)	63.8(5)	N(1)-Cu(1)-O(25)	99.3(5)
O(12)-W(2)-O(23)	66.2(5)	O(24)-Cu(1)-O(25)	104.6(5)
O(21)#1-W(2)-O(23)	44.0(5)	O(26)-Cu(1)-O(25)	89.0(5)
O(8)-W(3)-O(16)	102.3(6)	C(5)-N(1)-C(1)	118.9(14)
O(8)-W(3)-O(5)#1	101.0(5)	C(5)-N(1)-Cu(1)	113.7(11)
O(16)-W(3)-O(5)#1	156.6(5)	C(1)-N(1)-Cu(1)	123.7(11)
O(8)-W(3)-O(1)	100.9(5)	C(10)-N(2)-C(6)	118.3(14)
O(16)-W(3)-O(1)	85.7(5)	C(10)-N(2)-Cu(1)	115.0(12)
O(5)#1-W(3)-O(1)	90.6(4)	C(6)-N(2)-Cu(1)	126.7(12)
O(8)-W(3)-O(11)#1	103.5(5)	C(11)-N(3)-N(4)	105.7(11)
O(16)-W(3)-O(11)#1	87.4(5)	C(12)-N(4)-N(3)	107.5(12)
O(5)#1-W(3)-O(11)#1	86.5(5)	C(13)-N(5)-C(17)	123.3(17)
O(1)-W(3)-O(11)#1	155.5(5)	O(17)-W(5)-O(20)	63.4(5)
O(8)-W(3)-O(22)	156.2(6)	O(14)-W(5)-O(20)	62.0(5)
O(16)-W(3)-O(22)	61.2(5)	O(22)#1-W(5)-O(20)	49.5(5)
O(5)#1-W(3)-O(22)	96.2(6)	O(4)-W(6)-O(16)	100.5(5)
O(1)-W(3)-O(22)	95.2(6)	O(4)-W(6)-O(12)	100.0(5)
O(11)#1-W(3)-O(22)	61.1(5)	O(16)-W(6)-O(12)	159.5(5)
O(8)-W(3)-O(21)	154.7(6)	O(4)-W(6)-O(18)	99.6(6)
O(16)-W(3)-O(21)	96.6(6)	O(16)-W(6)-O(18)	87.4(5)
O(5)#1-W(3)-O(21)	61.4(5)	O(12)-W(6)-O(18)	89.6(5)
O(1)-W(3)-O(21)	63.7(5)	O(4)-W(6)-O(10)	100.2(5)
O(11)#1-W(3)-O(21)	93.9(6)	O(16)-W(6)-O(10)	87.9(5)
O(22)-W(3)-O(21)	49.1(6)	O(12)-W(6)-O(10)	88.1(4)
O(2)-W(4)-O(9)	100.9(5)	O(18)-W(6)-O(10)	160.1(5)
O(2)-W(4)-O(13)	101.4(6)	O(4)-W(6)-O(22)	154.2(6)
O(9)-W(4)-O(13)	157.6(6)	O(16)-W(6)-O(22)	62.1(6)
O(2)-W(4)-O(10)	99.8(5)	O(12)-W(6)-O(22)	98.6(5)
O(9)-W(4)-O(10)	87.9(4)	O(18)-W(6)-O(22)	62.7(6)
O(13)-W(4)-O(10)	88.6(5)	O(10)-W(6)-O(22)	98.1(5)
O(2)-W(4)-O(14)	101.4(6)	O(4)-W(6)-O(23)	158.3(6)
O(9)-W(4)-O(14)	88.0(5)	O(16)-W(6)-O(23)	95.5(6)
O(13)-W(4)-O(14)	87.3(5)	O(12)-W(6)-O(23)	64.6(5)

O(10)-W(4)-O(14)	158.9(5)	O(18)-W(6)-O(23)	95.7(6)
O(2)-W(4)-O(20)	157.1(6)	O(10)-W(6)-O(23)	65.6(5)
O(9)-W(4)-O(20)	95.8(5)	O(22)-W(6)-O(23)	47.6(5)
O(13)-W(4)-O(20)	62.6(6)	W(1)-O(1)-W(3)	137.9(5)
O(10)-W(4)-O(20)	96.3(5)	W(2)-O(5)-W(3)#1	137.1(6)
O(14)-W(4)-O(20)	63.5(5)	W(2)-O(7)-W(1)#1	136.0(7)
O(2)-W(4)-O(23)	158.0(6)	W(4)-O(9)-W(2)	138.3(7)
O(9)-W(4)-O(23)	62.8(6)	W(4)-O(10)-W(6)	135.4(5)
O(13)-W(4)-O(23)	95.6(6)	W(5)-O(11)-W(3)#1	140.3(7)
O(10)-W(4)-O(23)	66.7(5)	W(6)-O(12)-W(2)	135.2(7)
O(14)-W(4)-O(23)	93.1(6)	W(4)-O(13)-W(1)	139.0(7)
O(20)-W(4)-O(23)	44.9(6)	W(5)-O(14)-W(4)	137.9(7)
O(3)-W(5)-O(11)	102.1(5)	W(6)-O(16)-W(3)	138.9(7)
O(3)-W(5)-O(18)#1	100.7(5)	W(5)-O(17)-W(1)	138.1(8)
O(11)-W(5)-O(18)#1	87.0(5)	W(5)#1-O(18)-W(6)	137.3(8)
O(3)-W(5)-O(17)	100.7(5)	O(18)#1-W(5)-O(20)	97.9(6)
O(11)-W(5)-O(17)	157.2(6)	Si(1)-O(20)-O(23)	53.2(7)
O(18)#1-W(5)-O(17)	88.2(5)	Si(1)-O(20)-W(4)	123.7(9)
O(3)-W(5)-O(14)	100.5(5)	O(23)-O(20)-W(4)	70.6(8)
O(11)-W(5)-O(14)	88.0(5)	Si(1)-O(20)-W(1)	120.0(8)
O(18)#1-W(5)-O(14)	158.7(6)	O(23)-O(20)-W(1)	134.9(9)
O(17)-W(5)-O(14)	88.4(5)	W(4)-O(20)-W(1)	97.1(5)
O(3)-W(5)-O(22)#1	155.4(5)	Si(1)-O(20)-W(5)	118.7(7)
O(11)-W(5)-O(22)#1	61.6(5)	O(23)-O(20)-W(5)	128.9(9)
O(18)#1-W(5)-O(22)#1	62.3(6)	W(4)-O(20)-W(5)	96.3(5)
O(17)-W(5)-O(22)#1	96.5(6)	W(1)-O(20)-W(5)	94.7(6)
O(14)-W(5)-O(22)#1	97.3(6)	Si(1)-O(21)-O(23)#1	55.0(8)
O(3)-W(5)-O(20)	155.1(5)	Si(1)-O(21)-W(2)#1	125.7(8)
O(11)-W(5)-O(20)	95.2(6)	O(23)#1-O(21)-W(2)#1	70.6(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z #2 -x+1,-y+1,-z+2 #3 x,y+1,z #4 x,y-1,z

Table S3 The selected bond lengths (Å) for **2**

Si(1)-O(19)	1.40(2)	W(6)-O(13)	1.88(2)	C(9)-C(10)	1.30(3)
Si(1)-O(19)#1	1.40(2)	W(6)-O(16)	1.89(2)	C(10)-N(9)	1.38(2)
Si(1)-O(20)	1.61(2)	W(6)-O(2)#1	1.899(14)	C(11)-N(9)	1.31(3)
Si(1)-O(20)#1	1.61(2)	W(6)-O(21)#1	2.29(2)	C(11)-C(12)	1.36(3)
Si(1)-O(21)	1.68(3)	Cu(1)-N(12)#2	1.979(16)	C(13)-N(8)	1.37(2)
Si(1)-O(21)#1	1.68(3)	Cu(1)-N(9)	2.010(17)	C(13)-C(14)	1.38(3)
Si(1)-O(22)	1.69(3)	Cu(1)-N(5)#3	2.09(2)	C(14)-C(15)	1.35(3)
Si(1)-O(22)#1	1.69(3)	Cu(1)-N(8)	2.21(2)	C(15)-C(16)	1.40(2)
W(1)-O(6)	1.721(15)	Cu(2)-N(4)	2.023(16)	C(15)-C(18)	1.50(3)
W(1)-O(14)	1.88(2)	Cu(2)-N(7)#4	2.021(17)	C(16)-C(17)	1.38(3)
W(1)-O(18)	1.885(19)	Cu(2)-N(3)	2.029(18)	C(17)-N(8)	1.33(3)
W(1)-O(12)	1.940(15)	Cu(2)-N(6)	2.105(18)	C(18)-N(7)	1.39(3)

W(1)-O(3)	1.957(16)	O(2)-W(6)#1	1.899(14)	C(19)-N(6)	1.27(2)
W(1)-O(22)	2.26(3)	O(12)-W(5)#1	1.889(14)	C(19)-C(22)	1.47(3)
W(2)-O(4)	1.609(16)	O(14)-W(2)#1	1.905(19)	C(20)-C(21)	1.32(3)
W(2)-O(16)	1.86(2)	O(17)-W(3)#1	1.882(19)	C(20)-N(5)	1.42(3)
W(2)-O(17)	1.886(18)	O(19)-O(20)#1	1.46(3)	C(21)-C(22)	1.49(3)
W(2)-O(14)#1	1.905(19)	O(19)-O(21)	1.74(3)	C(22)-C(23)	1.39(3)
W(2)-O(9)	1.93(2)	O(20)-O(19)#1	1.46(3)	C(23)-C(24)	1.56(3)
W(2)-O(21)#1	2.47(3)	O(20)-W(5)#1	2.21(2)	C(24)-N(5)	1.26(3)
W(2)-O(22)#1	2.48(3)	O(20)-W(4)#1	2.50(2)	C(25)-N(4)	1.32(2)
W(3)-O(8)	1.688(14)	O(20)-W(3)#1	2.52(2)	C(25)-C(26)	1.38(2)
W(3)-O(18)	1.801(19)	O(21)-W(6)#1	2.29(2)	C(26)-C(27)	1.37(3)
W(3)-O(11)	1.870(16)	O(21)-W(4)#1	2.36(2)	C(27)-C(28)	1.41(3)
W(3)-O(17)#1	1.882(19)	O(21)-W(2)#1	2.47(3)	C(27)-C(30)	1.47(3)
W(3)-O(5)	1.938(19)	O(22)-W(2)#1	2.48(3)	C(28)-C(29)	1.37(2)
W(3)-O(22)	2.35(2)	O(23)-C(30)	1.34(3)	C(29)-N(4)	1.30(2)
W(3)-O(20)#1	2.52(2)	O(23)-C(36)#5	1.36(2)	C(30)-N(1)#5	1.35(3)
W(4)-O(10)	1.672(14)	O(24)-C(18)	1.32(2)	C(31)-N(3)	1.31(2)
W(4)-O(7)	1.852(17)	O(24)-C(19)	1.33(2)	C(31)-C(32)	1.37(3)
W(4)-O(11)	1.903(17)	O(25)-C(7)	1.32(2)	C(32)-C(33)	1.36(3)
W(4)-O(9)	1.90(2)	O(25)-C(6)	1.33(2)	C(33)-C(36)	1.41(3)
W(4)-O(13)	1.99(2)	O(1W)-O(2W)	1.39(3)	C(33)-C(34)	1.41(3)
W(4)-O(21)#1	2.36(2)	C(1)-N(12)	1.31(2)	C(34)-C(35)	1.38(3)
W(4)-O(20)#1	2.50(2)	C(1)-C(2)	1.39(2)	C(35)-N(3)	1.31(3)
W(5)-O(15)	1.673(18)	C(2)-C(3)	1.36(3)	C(36)-N(2)	1.34(3)
W(5)-O(5)	1.83(2)	C(3)-C(4)	1.33(3)	C(36)-O(23)#2	1.36(2)
W(5)-O(2)	1.874(14)	C(3)-C(6)	1.43(3)	N(1)-C(30)#2	1.35(3)
W(5)-O(12)#1	1.889(15)	C(5)-N(12)	1.32(3)	N(1)-N(2)	1.38(2)
W(5)-O(7)	1.933(18)	C(6)-N(11)	1.36(3)	N(5)-Cu(1)#3	2.09(2)
W(5)-O(20)#1	2.21(2)	C(7)-N(10)	1.33(3)	N(6)-N(7)	1.41(2)
W(5)-O(19)	2.39(2)	C(7)-C(8)	1.48(3)	N(7)-Cu(2)#4	2.021(17)
W(6)-O(1)	1.691(15)	C(8)-C(9)	1.36(3)	N(10)-N(11)	1.38(2)
W(6)-O(3)	1.814(16)	C(8)-C(12)	1.44(3)	N(12)-Cu(1)#5	1.979(16)

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

Table S4 The selected bond angles (°) for **2**

O(19)-Si(1)-O(19)#1	180.0(10)	N(9)-Cu(1)-N(5)#3	108.0(8)
O(19)-Si(1)-O(20)	122.3(12)	N(12)#2-Cu(1)-N(8)	118.2(7)
O(19)#1-Si(1)-O(20)	57.7(12)	N(9)-Cu(1)-N(8)	102.5(7)
O(19)-Si(1)-O(20)#1	57.7(12)	N(5)#3-Cu(1)-N(8)	88.1(8)
O(19)#1-Si(1)-O(20)#1	122.3(12)	N(4)-Cu(2)-N(7)#4	112.1(6)
O(20)-Si(1)-O(20)#1	180.0(18)	N(4)-Cu(2)-N(3)	125.7(7)
O(19)-Si(1)-O(21)	68.1(13)	N(7)#4-Cu(2)-N(3)	103.0(7)
O(19)#1-Si(1)-O(21)	111.9(13)	N(4)-Cu(2)-N(6)	102.7(7)
O(20)-Si(1)-O(21)	74.0(12)	N(7)#4-Cu(2)-N(6)	105.0(6)
O(20)#1-Si(1)-O(21)	106.0(12)	N(3)-Cu(2)-N(6)	106.7(7)

O(19)-Si(1)-O(21)#1	111.9(13)	W(5)-O(2)-W(6)#1	138.8(9)
O(19)#1-Si(1)-O(21)#1	68.1(13)	W(6)-O(3)-W(1)	138.4(8)
O(20)-Si(1)-O(21)#1	106.0(12)	W(5)-O(5)-W(3)	137.8(11)
O(20)#1-Si(1)-O(21)#1	74.0(12)	W(4)-O(7)-W(5)	137.2(10)
O(21)-Si(1)-O(21)#1	180.000(2)	W(4)-O(9)-W(2)	134.6(12)
O(19)-Si(1)-O(22)	108.4(13)	W(3)-O(11)-W(4)	138.5(9)
O(19)#1-Si(1)-O(22)	71.6(13)	W(5)#1-O(12)-W(1)	135.7(8)
O(20)-Si(1)-O(22)	104.9(12)	W(6)-O(13)-W(4)	130.5(11)
O(20)#1-Si(1)-O(22)	75.1(12)	W(1)-O(14)-W(2)#1	138.3(11)
O(21)-Si(1)-O(22)	78.9(12)	W(2)-O(16)-W(6)	141.1(13)
O(21)#1-Si(1)-O(22)	101.1(12)	W(3)#1-O(17)-W(2)	138.7(11)
O(19)-Si(1)-O(22)#1	71.6(13)	W(3)-O(18)-W(1)	143.1(12)
O(19)#1-Si(1)-O(22)#1	108.4(13)	Si(1)-O(19)-O(20)#1	68.2(14)
O(20)-Si(1)-O(22)#1	75.1(12)	Si(1)-O(19)-O(21)	63.4(13)
O(20)#1-Si(1)-O(22)#1	104.9(12)	O(20)#1-O(19)-O(21)	110(2)
O(21)-Si(1)-O(22)#1	101.1(12)	Si(1)-O(19)-W(5)	132.9(14)
O(21)#1-Si(1)-O(22)#1	78.9(12)	O(20)#1-O(19)-W(5)	64.7(13)
O(22)-Si(1)-O(22)#1	180.0(18)	O(21)-O(19)-W(5)	134.8(16)
O(6)-W(1)-O(14)	102.6(9)	O(19)#1-O(20)-Si(1)	54.1(13)
O(6)-W(1)-O(18)	105.0(8)	O(19)#1-O(20)-W(5)#1	78.5(14)
O(14)-W(1)-O(18)	89.2(8)	Si(1)-O(20)-W(5)#1	132.7(13)
O(6)-W(1)-O(12)	100.0(6)	O(19)#1-O(20)-W(4)#1	137.4(18)
O(14)-W(1)-O(12)	86.4(8)	Si(1)-O(20)-W(4)#1	117.0(12)
O(18)-W(1)-O(12)	155.0(8)	W(5)#1-O(20)-W(4)#1	96.7(8)
O(6)-W(1)-O(3)	102.2(7)	O(19)#1-O(20)-W(3)#1	133.3(17)
O(14)-W(1)-O(3)	155.2(8)	Si(1)-O(20)-W(3)#1	115.5(12)
O(18)-W(1)-O(3)	84.9(7)	W(5)#1-O(20)-W(3)#1	95.9(9)
O(12)-W(1)-O(3)	88.8(6)	W(4)#1-O(20)-W(3)#1	89.2(7)
O(6)-W(1)-O(22)	158.1(9)	Si(1)-O(21)-O(19)	48.4(11)
O(14)-W(1)-O(22)	64.6(9)	Si(1)-O(21)-W(6)#1	125.2(13)
O(18)-W(1)-O(22)	59.3(9)	O(19)-O(21)-W(6)#1	77.0(12)
O(12)-W(1)-O(22)	96.9(7)	Si(1)-O(21)-W(4)#1	121.2(13)
O(3)-W(1)-O(22)	91.9(8)	O(19)-O(21)-W(4)#1	142.6(17)
O(4)-W(2)-O(16)	104.9(9)	W(6)#1-O(21)-W(4)#1	98.3(9)
O(4)-W(2)-O(17)	102.6(9)	Si(1)-O(21)-W(2)#1	115.4(12)
O(16)-W(2)-O(17)	88.2(8)	O(19)-O(21)-W(2)#1	123.2(15)
O(4)-W(2)-O(14)#1	101.0(8)	W(6)#1-O(21)-W(2)#1	95.9(9)
O(16)-W(2)-O(14)#1	153.8(10)	W(4)#1-O(21)-W(2)#1	94.1(9)
O(17)-W(2)-O(14)#1	90.3(8)	Si(1)-O(22)-W(1)	126.0(13)
O(4)-W(2)-O(9)	98.6(9)	Si(1)-O(22)-W(3)	120.7(13)
O(16)-W(2)-O(9)	87.7(9)	W(1)-O(22)-W(3)	98.6(10)
O(17)-W(2)-O(9)	158.7(9)	Si(1)-O(22)-W(2)#1	114.5(12)
O(14)#1-W(2)-O(9)	84.2(8)	W(1)-O(22)-W(2)#1	96.3(10)
O(4)-W(2)-O(21)#1	155.4(8)	W(3)-O(22)-W(2)#1	93.9(9)
O(16)-W(2)-O(21)#1	59.4(9)	C(30)-O(23)-C(36)#5	103.8(18)
O(17)-W(2)-O(21)#1	95.9(8)	C(18)-O(24)-C(19)	103.1(17)

O(14)#1-W(2)-O(21)#1	94.8(9)	C(7)-O(25)-C(6)	106.1(19)
O(9)-W(2)-O(21)#1	64.2(9)	N(12)-C(1)-C(2)	124(2)
O(4)-W(2)-O(22)#1	153.2(8)	C(3)-C(2)-C(1)	119(2)
O(16)-W(2)-O(22)#1	97.0(9)	C(4)-C(3)-C(2)	117(2)
O(17)-W(2)-O(22)#1	62.1(8)	C(4)-C(3)-C(6)	125(2)
O(14)#1-W(2)-O(22)#1	59.7(9)	C(2)-C(3)-C(6)	118(2)
O(9)-W(2)-O(22)#1	97.7(9)	C(3)-C(4)-C(5)	122(2)
O(21)#1-W(2)-O(22)#1	51.2(8)	N(12)-C(5)-C(4)	122(2)
O(8)-W(3)-O(18)	104.4(8)	O(25)-C(6)-N(11)	111(2)
O(8)-W(3)-O(11)	100.6(8)	O(25)-C(6)-C(3)	126(2)
O(18)-W(3)-O(11)	90.8(8)	N(11)-C(6)-C(3)	123(2)
O(8)-W(3)-O(17)#1	101.9(8)	O(25)-C(7)-N(10)	110.9(19)
O(18)-W(3)-O(17)#1	88.5(8)	O(25)-C(7)-C(8)	121(2)
O(11)-W(3)-O(17)#1	156.9(8)	N(10)-C(7)-C(8)	129(2)
O(8)-W(3)-O(5)	100.4(7)	C(9)-C(8)-C(12)	119(2)
O(18)-W(3)-O(5)	154.9(9)	C(9)-C(8)-C(7)	119.6(19)
O(11)-W(3)-O(5)	87.5(8)	C(12)-C(8)-C(7)	122(2)
O(17)#1-W(3)-O(5)	83.5(8)	C(10)-C(9)-C(8)	116(2)
O(8)-W(3)-O(22)	156.9(8)	C(9)-C(10)-N(9)	131(2)
O(18)-W(3)-O(22)	58.3(9)	N(9)-C(11)-C(12)	126(2)
O(11)-W(3)-O(22)	95.2(8)	C(11)-C(12)-C(8)	117(2)
O(17)#1-W(3)-O(22)	65.0(9)	N(8)-C(13)-C(14)	121(2)
O(5)-W(3)-O(22)	96.9(8)	C(15)-C(14)-C(13)	117(2)
O(8)-W(3)-O(20)#1	154.3(7)	C(14)-C(15)-C(16)	124(2)
O(18)-W(3)-O(20)#1	97.8(9)	C(14)-C(15)-C(18)	118.3(19)
O(11)-W(3)-O(20)#1	66.1(7)	C(16)-C(15)-C(18)	118(2)
O(17)#1-W(3)-O(20)#1	91.1(8)	C(17)-C(16)-C(15)	115(2)
O(5)-W(3)-O(20)#1	58.8(8)	N(8)-C(17)-C(16)	123(2)
O(22)-W(3)-O(20)#1	48.6(8)	O(24)-C(18)-N(7)	112.2(18)
O(10)-W(4)-O(7)	102.1(7)	O(24)-C(18)-C(15)	122(2)
O(10)-W(4)-O(11)	101.5(8)	N(7)-C(18)-C(15)	125.3(19)
O(7)-W(4)-O(11)	87.4(8)	N(6)-C(19)-O(24)	115.4(19)
O(10)-W(4)-O(9)	98.6(9)	N(6)-C(19)-C(22)	128(2)
O(7)-W(4)-O(9)	91.5(8)	O(24)-C(19)-C(22)	116.8(19)
O(11)-W(4)-O(9)	159.7(8)	C(21)-C(20)-N(5)	127(3)
O(10)-W(4)-O(13)	96.2(8)	C(20)-C(21)-C(22)	115(3)
O(7)-W(4)-O(13)	161.5(8)	C(23)-C(22)-C(19)	117(2)
O(11)-W(4)-O(13)	86.2(8)	C(23)-C(22)-C(21)	120(2)
O(9)-W(4)-O(13)	88.5(9)	C(19)-C(22)-C(21)	122(2)
O(10)-W(4)-O(21)#1	154.8(8)	N(5)-C(24)-C(23)	120(3)
O(7)-W(4)-O(21)#1	99.1(8)	N(4)-C(25)-C(26)	125(2)
O(11)-W(4)-O(21)#1	93.1(8)	C(27)-C(26)-C(25)	120(2)
O(9)-W(4)-O(21)#1	67.1(9)	C(26)-C(27)-C(28)	115.3(19)
O(13)-W(4)-O(21)#1	64.0(8)	C(26)-C(27)-C(30)	122(2)
O(10)-W(4)-O(20)#1	157.4(7)	C(28)-C(27)-C(30)	123(2)
O(7)-W(4)-O(20)#1	60.1(7)	C(29)-C(28)-C(27)	119(2)

O(11)-W(4)-O(20)#1	66.2(7)	N(4)-C(29)-C(28)	125(2)
O(9)-W(4)-O(20)#1	95.8(9)	O(23)-C(30)-N(1)#5	111(2)
O(13)-W(4)-O(20)#1	101.5(8)	O(23)-C(30)-C(27)	122(2)
O(21)#1-W(4)-O(20)#1	47.8(8)	N(1)#5-C(30)-C(27)	126(2)
O(15)-W(5)-O(5)	103.9(9)	N(3)-C(31)-C(32)	121(3)
O(15)-W(5)-O(2)	99.6(8)	C(33)-C(32)-C(31)	126(3)
O(5)-W(5)-O(2)	91.3(8)	C(32)-C(33)-C(36)	123(2)
O(15)-W(5)-O(12)#1	96.2(8)	C(32)-C(33)-C(34)	112(2)
O(5)-W(5)-O(12)#1	159.8(7)	C(36)-C(33)-C(34)	124(2)
O(2)-W(5)-O(12)#1	87.7(7)	C(35)-C(34)-C(33)	118(2)
O(15)-W(5)-O(7)	101.4(8)	N(3)-C(35)-C(34)	126(2)
O(5)-W(5)-O(7)	88.3(8)	N(2)-C(36)-O(23)#2	112.4(19)
O(2)-W(5)-O(7)	158.5(7)	N(2)-C(36)-C(33)	128(2)
O(12)#1-W(5)-O(7)	85.3(7)	O(23)#2-C(36)-C(33)	119(2)
O(15)-W(5)-O(20)#1	163.2(9)	C(30)#2-N(1)-N(2)	107(2)
O(5)-W(5)-O(20)#1	66.8(9)	C(36)-N(2)-N(1)	105.2(18)
O(2)-W(5)-O(20)#1	94.8(8)	C(31)-N(3)-C(35)	116(2)
O(12)#1-W(5)-O(20)#1	93.2(8)	C(31)-N(3)-Cu(2)	117.2(15)
O(7)-W(5)-O(20)#1	65.4(8)	C(35)-N(3)-Cu(2)	126.2(15)
O(15)-W(5)-O(19)	159.9(9)	C(29)-N(4)-C(25)	115.8(19)
O(5)-W(5)-O(19)	91.4(8)	C(29)-N(4)-Cu(2)	125.4(15)
O(2)-W(5)-O(19)	66.5(7)	C(25)-N(4)-Cu(2)	116.8(15)
O(12)#1-W(5)-O(19)	69.8(7)	C(24)-N(5)-C(20)	120(2)
O(7)-W(5)-O(19)	92.1(8)	C(24)-N(5)-Cu(1)#3	118.2(19)
O(20)#1-W(5)-O(19)	36.8(8)	C(20)-N(5)-Cu(1)#3	115.5(19)
O(1)-W(6)-O(3)	101.9(9)	C(19)-N(6)-N(7)	107.1(18)
O(1)-W(6)-O(13)	97.3(8)	C(19)-N(6)-Cu(2)	124.0(15)
O(3)-W(6)-O(13)	89.3(8)	N(7)-N(6)-Cu(2)	127.3(13)
O(1)-W(6)-O(16)	102.4(10)	C(18)-N(7)-N(6)	102.2(16)
O(3)-W(6)-O(16)	155.5(8)	C(18)-N(7)-Cu(2)#4	126.1(14)
O(13)-W(6)-O(16)	90.1(9)	N(6)-N(7)-Cu(2)#4	127.4(14)
O(1)-W(6)-O(2)#1	100.8(7)	C(17)-N(8)-C(13)	119(2)
O(3)-W(6)-O(2)#1	88.5(6)	C(17)-N(8)-Cu(1)	118.5(15)
O(13)-W(6)-O(2)#1	161.8(8)	C(13)-N(8)-Cu(1)	118.3(16)
O(16)-W(6)-O(2)#1	84.4(8)	C(11)-N(9)-C(10)	111(2)
O(1)-W(6)-O(21)#1	157.2(10)	C(11)-N(9)-Cu(1)	126.0(16)
O(3)-W(6)-O(21)#1	94.6(8)	C(10)-N(9)-Cu(1)	122.0(16)
O(13)-W(6)-O(21)#1	67.0(9)	C(7)-N(10)-N(11)	107.6(18)
O(16)-W(6)-O(21)#1	62.9(9)	C(6)-N(11)-N(10)	104.1(19)
O(2)#1-W(6)-O(21)#1	95.2(8)	C(1)-N(12)-C(5)	116.0(19)
N(12)#2-Cu(1)-N(9)	130.2(7)	C(1)-N(12)-Cu(1)#5	124.4(16)
N(12)#2-Cu(1)-N(5)#3	101.2(8)	C(5)-N(12)-Cu(1)#5	117.5(15)

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

Table S5 The selected bond lengths (Å) for **3**

Si(1)-O(20)#1	1.55(4)	W(4)-O(18)	2.42(4)	O(24)-C(6)	1.38(4)
Si(1)-O(20)	1.55(4)	W(4)-O(16)#1	2.44(5)	C(1)-N(1)	1.28(5)
Si(1)-O(16)	1.63(5)	W(5)-O(8)	1.68(2)	C(1)-C(2)	1.45(6)
Si(1)-O(16)#1	1.63(5)	W(5)-O(10)#1	1.90(4)	C(2)-C(3)	1.30(6)
Si(1)-O(15)	1.63(4)	W(5)-O(12)	1.91(4)	C(3)-C(4)	1.43(5)
Si(1)-O(15)#1	1.63(4)	W(5)-O(17)	1.92(4)	C(4)-C(5)	1.32(5)
Si(1)-O(18)#1	1.64(4)	W(5)-O(11)	1.93(3)	C(4)-C(6)	1.46(5)
Si(1)-O(18)	1.64(4)	W(5)-O(16)	2.38(5)	C(5)-N(1)	1.43(4)
W(1)-O(1)	1.70(2)	W(5)-O(15)#1	2.40(4)	C(6)-N(2)	1.28(5)
W(1)-O(19)#1	1.81(4)	W(6)-O(2)	1.64(3)	C(7)-N(3)	1.29(5)
W(1)-O(17)#1	1.89(4)	W(6)-O(12)	1.84(4)	C(7)-C(9)	1.41(5)
W(1)-O(7)	1.89(3)	W(6)-O(14)	1.86(4)	C(8)-C(9)	1.35(5)
W(1)-O(3)	1.91(3)	W(6)-O(22)	1.92(3)	C(8)-N(4)	1.39(5)
W(1)-O(15)	2.34(4)	W(6)-O(19)	1.93(3)	C(9)-C(10)	1.41(6)
W(1)-O(20)	2.44(4)	W(6)-O(18)	2.39(4)	C(10)-C(11)	1.39(5)
W(2)-O(5)	1.70(3)	W(6)-O(15)#1	2.42(4)	C(11)-C(12)	1.42(6)
W(2)-O(11)	1.85(3)	Cu(1)-N(8)	1.89(3)	C(12)-N(4)	1.25(5)
W(2)-O(4)	1.87(3)	Cu(1)-N(1)	1.91(3)	C(13)-C(14)	1.33(6)
W(2)-O(13)	1.89(4)	Cu(1)-O(1)	2.39(2)	C(13)-N(5)	1.34(5)
W(2)-O(7)	1.91(3)	Cu(2)-N(5)	1.88(3)	C(14)-C(15)	1.35(5)
W(2)-O(16)	2.34(5)	Cu(2)-N(4)	1.89(3)	C(15)-C(16)	1.46(5)
W(2)-O(20)	2.45(5)	O(10)-W(5)#1	1.90(4)	C(16)-C(17)	1.39(5)
W(3)-O(21)	1.67(3)	O(13)-W(4)#1	1.88(4)	C(16)-C(18)	1.42(5)
W(3)-O(6)	1.87(4)	O(15)-O(20)	1.81(6)	C(17)-N(5)	1.37(5)
W(3)-O(3)	1.88(3)	O(15)-W(5)#1	2.40(4)	C(18)-N(6)	1.33(5)
W(3)-O(4)	1.89(3)	O(15)-W(6)#1	2.42(4)	C(19)-N(7)	1.18(5)
W(3)-O(14)	1.90(3)	O(16)-O(20)	1.82(7)	C(19)-C(21)	1.45(5)
W(3)-O(18)	2.35(4)	O(16)-W(4)#1	2.44(5)	C(20)-N(8)	1.32(4)
W(3)-O(20)	2.40(4)	O(17)-W(1)#1	1.89(4)	C(20)-C(21)	1.36(5)
W(4)-O(9)	1.67(3)	O(18)-O(20)	1.78(6)	C(21)-C(22)	1.43(5)
W(4)-O(10)	1.85(4)	O(19)-W(1)#1	1.81(3)	C(22)-C(23)	1.43(6)
W(4)-O(22)	1.86(3)	O(23)-C(18)	1.32(4)	C(24)-N(8)	1.37(5)
W(4)-O(6)	1.87(4)	O(23)-C(19)	1.43(4)	N(2)-N(3)	1.38(5)
W(4)-O(13)#1	1.88(4)	O(24)-C(7)	1.34(4)	N(6)-N(7)	1.44(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1

Table S6 The selected bond angles (º) for **3**

O(20)#1-Si(1)-O(20)	180.000(11)	O(12)-W(6)-O(19)	88.0(15)
O(20)#1-Si(1)-O(16)	110(2)	O(14)-W(6)-O(19)	155(2)
O(20)-Si(1)-O(16)	70(2)	O(22)-W(6)-O(19)	84.4(17)
O(20)#1-Si(1)-O(16)#1	70(2)	O(2)-W(6)-O(18)	157.4(14)
O(20)-Si(1)-O(16)#1	110(2)	O(12)-W(6)-O(18)	93.2(14)
O(16)-Si(1)-O(16)#1	180(2)	O(14)-W(6)-O(18)	62.9(15)
O(20)#1-Si(1)-O(15)	111(2)	O(22)-W(6)-O(18)	64.2(15)

O(20)-Si(1)-O(15)	69(2)	O(19)-W(6)-O(18)	92.7(18)
O(16)-Si(1)-O(15)	108(2)	O(2)-W(6)-O(15)#1	156.1(15)
O(16)#1-Si(1)-O(15)	72(2)	O(12)-W(6)-O(15)#1	62.4(15)
O(20)#1-Si(1)-O(15)#1	69(2)	O(14)-W(6)-O(15)#1	96.7(17)
O(20)-Si(1)-O(15)#1	111(2)	O(22)-W(6)-O(15)#1	94.1(18)
O(16)-Si(1)-O(15)#1	72(2)	O(19)-W(6)-O(15)#1	59.7(18)
O(16)#1-Si(1)-O(15)#1	108(2)	O(18)-W(6)-O(15)#1	46.4(14)
O(15)-Si(1)-O(15)#1	180(2)	N(8)-Cu(1)-N(1)	164.6(13)
O(20)#1-Si(1)-O(18)#1	68(2)	N(8)-Cu(1)-O(1)	100.2(11)
O(20)-Si(1)-O(18)#1	112(2)	N(1)-Cu(1)-O(1)	95.2(11)
O(16)-Si(1)-O(18)#1	74(2)	N(5)-Cu(2)-N(4)	167.2(13)
O(16)#1-Si(1)-O(18)#1	106(2)	W(1)-O(1)-Cu(1)	159.2(13)
O(15)-Si(1)-O(18)#1	71(2)	W(3)-O(3)-W(1)	137.8(16)
O(15)#1-Si(1)-O(18)#1	109(2)	W(2)-O(4)-W(3)	140.4(19)
O(20)#1-Si(1)-O(18)	112(2)	W(4)-O(6)-W(3)	140(2)
O(20)-Si(1)-O(18)	68(2)	W(1)-O(7)-W(2)	135(2)
O(16)-Si(1)-O(18)	106(2)	W(4)-O(10)-W(5)#1	141(2)
O(16)#1-Si(1)-O(18)	74(2)	W(2)-O(11)-W(5)	136(3)
O(15)-Si(1)-O(18)	109(2)	W(6)-O(12)-W(5)	141(2)
O(15)#1-Si(1)-O(18)	71(2)	W(4)#1-O(13)-W(2)	138(3)
O(18)#1-Si(1)-O(18)	180(2)	W(6)-O(14)-W(3)	138(2)
O(1)-W(1)-O(19)#1	104.0(18)	Si(1)-O(15)-O(20)	53.1(19)
O(1)-W(1)-O(17)#1	100.1(14)	Si(1)-O(15)-W(1)	124(2)
O(19)#1-W(1)-O(17)#1	87.3(15)	O(20)-O(15)-W(1)	70(2)
O(1)-W(1)-O(7)	99.1(16)	Si(1)-O(15)-W(5)#1	120(2)
O(19)#1-W(1)-O(7)	89.5(16)	O(20)-O(15)-W(5)#1	129(3)
O(17)#1-W(1)-O(7)	160.8(16)	W(1)-O(15)-W(5)#1	96.2(15)
O(1)-W(1)-O(3)	99.4(12)	Si(1)-O(15)-W(6)#1	121(2)
O(19)#1-W(1)-O(3)	156.5(18)	O(20)-O(15)-W(6)#1	135(3)
O(17)#1-W(1)-O(3)	86.2(14)	W(1)-O(15)-W(6)#1	95.8(15)
O(7)-W(1)-O(3)	89.3(13)	W(5)#1-O(15)-W(6)#1	94.2(15)
O(1)-W(1)-O(15)	158.8(14)	Si(1)-O(16)-O(20)	53(2)
O(19)#1-W(1)-O(15)	62.6(18)	Si(1)-O(16)-W(2)	124(3)
O(17)#1-W(1)-O(15)	64.6(15)	O(20)-O(16)-W(2)	71(2)
O(7)-W(1)-O(15)	97.2(17)	Si(1)-O(16)-W(5)	121(3)
O(3)-W(1)-O(15)	94.3(13)	O(20)-O(16)-W(5)	134(3)
O(1)-W(1)-O(20)	156.4(14)	W(2)-O(16)-W(5)	95.9(18)
O(19)#1-W(1)-O(20)	95(2)	Si(1)-O(16)-W(4)#1	119(3)
O(17)#1-W(1)-O(20)	94.8(15)	O(20)-O(16)-W(4)#1	130(3)
O(7)-W(1)-O(20)	66.7(15)	W(2)-O(16)-W(4)#1	94.9(17)
O(3)-W(1)-O(20)	63.2(13)	W(5)-O(16)-W(4)#1	94.3(17)
O(15)-W(1)-O(20)	44.6(15)	W(1)#1-O(17)-W(5)	136(2)
O(5)-W(2)-O(11)	99.6(19)	Si(1)-O(18)-O(20)	53.7(19)
O(5)-W(2)-O(4)	101.1(14)	Si(1)-O(18)-W(3)	123(2)
O(11)-W(2)-O(4)	90.4(14)	O(20)-O(18)-W(3)	69.5(19)
O(5)-W(2)-O(13)	102.5(19)	Si(1)-O(18)-W(6)	122(2)

O(11)-W(2)-O(13)	87.7(14)	O(20)-O(18)-W(6)	132(2)
O(4)-W(2)-O(13)	156(2)	W(3)-O(18)-W(6)	95.6(14)
O(5)-W(2)-O(7)	99.6(17)	Si(1)-O(18)-W(4)	120(2)
O(11)-W(2)-O(7)	161(2)	O(20)-O(18)-W(4)	132(2)
O(4)-W(2)-O(7)	89.5(12)	W(3)-O(18)-W(4)	95.0(14)
O(13)-W(2)-O(7)	84.7(15)	W(6)-O(18)-W(4)	94.2(14)
O(5)-W(2)-O(16)	158.8(17)	W(1)#1-O(19)-W(6)	141(3)
O(11)-W(2)-O(16)	64.9(19)	Si(1)-O(20)-O(18)	58.3(19)
O(4)-W(2)-O(16)	93.6(17)	Si(1)-O(20)-O(15)	57(2)
O(13)-W(2)-O(16)	64(2)	O(18)-O(20)-O(15)	96(3)
O(7)-W(2)-O(16)	95.7(19)	Si(1)-O(20)-O(16)	57(2)
O(5)-W(2)-O(20)	156.7(15)	O(18)-O(20)-O(16)	93(3)
O(11)-W(2)-O(20)	96.8(19)	O(15)-O(20)-O(16)	93(3)
O(4)-W(2)-O(20)	62.3(15)	Si(1)-O(20)-W(3)	125(2)
O(13)-W(2)-O(20)	95(2)	O(18)-O(20)-W(3)	66.5(19)
O(7)-W(2)-O(20)	66.0(16)	O(15)-O(20)-W(3)	131(3)
O(16)-W(2)-O(20)	44.4(16)	O(16)-O(20)-W(3)	131(3)
O(21)-W(3)-O(6)	101.3(14)	Si(1)-O(20)-W(1)	122(2)
O(21)-W(3)-O(3)	100.9(15)	O(18)-O(20)-W(1)	134(3)
O(6)-W(3)-O(3)	87.6(14)	O(15)-O(20)-W(1)	64.9(19)
O(21)-W(3)-O(4)	105.0(15)	O(16)-O(20)-W(1)	127(3)
O(6)-W(3)-O(4)	153.7(16)	W(3)-O(20)-W(1)	94.1(15)
O(3)-W(3)-O(4)	87.9(12)	Si(1)-O(20)-W(2)	122(2)
O(21)-W(3)-O(14)	101.7(19)	O(18)-O(20)-W(2)	129(3)
O(6)-W(3)-O(14)	90.7(15)	O(15)-O(20)-W(2)	129(3)
O(3)-W(3)-O(14)	157.2(17)	O(16)-O(20)-W(2)	65(2)
O(4)-W(3)-O(14)	83.6(15)	W(3)-O(20)-W(2)	93.5(15)
O(21)-W(3)-O(18)	155.9(15)	W(1)-O(20)-W(2)	92.0(15)
O(6)-W(3)-O(18)	62.5(14)	W(4)-O(22)-W(6)	137(2)
O(3)-W(3)-O(18)	96.2(13)	C(18)-O(23)-C(19)	104(3)
O(4)-W(3)-O(18)	92.3(15)	C(7)-O(24)-C(6)	103(3)
O(14)-W(3)-O(18)	63.2(16)	N(1)-C(1)-C(2)	124(4)
O(21)-W(3)-O(20)	160.1(15)	C(3)-C(2)-C(1)	116(4)
O(6)-W(3)-O(20)	91.8(15)	C(2)-C(3)-C(4)	121(4)
O(3)-W(3)-O(20)	64.3(14)	C(5)-C(4)-C(3)	120(4)
O(4)-W(3)-O(20)	63.1(15)	C(5)-C(4)-C(6)	121(3)
O(14)-W(3)-O(20)	93.1(18)	C(3)-C(4)-C(6)	118(4)
O(18)-W(3)-O(20)	44.0(14)	C(4)-C(5)-N(1)	120(3)
O(9)-W(4)-O(10)	101.4(16)	N(2)-C(6)-O(24)	112(3)
O(9)-W(4)-O(22)	101.8(18)	N(2)-C(6)-C(4)	131(4)
O(10)-W(4)-O(22)	156.6(19)	O(24)-C(6)-C(4)	117(3)
O(9)-W(4)-O(6)	102.0(15)	N(3)-C(7)-O(24)	110(3)
O(10)-W(4)-O(6)	81.2(16)	N(3)-C(7)-C(9)	128(4)
O(22)-W(4)-O(6)	90.3(15)	O(24)-C(7)-C(9)	122(3)
O(9)-W(4)-O(13)#1	103(2)	C(9)-C(8)-N(4)	123(3)
O(10)-W(4)-O(13)#1	88.0(16)	C(8)-C(9)-C(10)	119(4)

O(22)-W(4)-O(13)#1	90.7(17)	C(8)-C(9)-C(7)	122(4)
O(6)-W(4)-O(13)#1	155(2)	C(10)-C(9)-C(7)	119(4)
O(9)-W(4)-O(18)	156.3(14)	C(11)-C(10)-C(9)	117(4)
O(10)-W(4)-O(18)	92.6(15)	C(10)-C(11)-C(12)	118(4)
O(22)-W(4)-O(18)	64.3(16)	N(4)-C(12)-C(11)	124(4)
O(6)-W(4)-O(18)	61.0(14)	C(14)-C(13)-N(5)	123(3)
O(13)#1-W(4)-O(18)	97(2)	C(13)-C(14)-C(15)	123(4)
O(9)-W(4)-O(16)#1	156.0(16)	C(14)-C(15)-C(16)	116(4)
O(10)-W(4)-O(16)#1	61.8(17)	C(17)-C(16)-C(18)	120(3)
O(22)-W(4)-O(16)#1	97(2)	C(17)-C(16)-C(15)	119(3)
O(6)-W(4)-O(16)#1	92.6(16)	C(18)-C(16)-C(15)	121(3)
O(13)#1-W(4)-O(16)#1	62(2)	N(5)-C(17)-C(16)	121(3)
O(18)-W(4)-O(16)#1	47.4(15)	O(23)-C(18)-N(6)	112(3)
O(8)-W(5)-O(10)#1	103.8(16)	O(23)-C(18)-C(16)	121(3)
O(8)-W(5)-O(12)	102.1(15)	N(6)-C(18)-C(16)	126(3)
O(10)#1-W(5)-O(12)	154.0(16)	N(7)-C(19)-O(23)	110(4)
O(8)-W(5)-O(17)	100.0(14)	N(7)-C(19)-C(21)	133(4)
O(10)#1-W(5)-O(17)	90.8(16)	O(23)-C(19)-C(21)	117(3)
O(12)-W(5)-O(17)	87.2(15)	N(8)-C(20)-C(21)	124(3)
O(8)-W(5)-O(11)	99.5(18)	C(20)-C(21)-C(22)	120(3)
O(10)#1-W(5)-O(11)	87.6(15)	C(20)-C(21)-C(19)	126(3)
O(12)-W(5)-O(11)	85.6(15)	C(22)-C(21)-C(19)	114(3)
O(17)-W(5)-O(11)	160.2(18)	C(21)-C(22)-C(23)	114(4)
O(8)-W(5)-O(16)	157.0(16)	C(24)-C(23)-C(22)	120(4)
O(10)#1-W(5)-O(16)	62.8(17)	C(23)-C(24)-N(8)	126(4)
O(12)-W(5)-O(16)	91.9(16)	C(1)-N(1)-C(5)	117(3)
O(17)-W(5)-O(16)	98.8(16)	C(1)-N(1)-Cu(1)	127(3)
O(11)-W(5)-O(16)	63.1(18)	C(5)-N(1)-Cu(1)	115(2)
O(8)-W(5)-O(15)#1	155.8(14)	C(6)-N(2)-N(3)	105(3)
O(10)#1-W(5)-O(15)#1	94.1(16)	C(7)-N(3)-N(2)	110(3)
O(12)-W(5)-O(15)#1	62.1(15)	C(12)-N(4)-C(8)	118(3)
O(17)-W(5)-O(15)#1	63.0(15)	C(12)-N(4)-Cu(2)	119(3)
O(11)-W(5)-O(15)#1	97.4(18)	C(8)-N(4)-Cu(2)	118(2)
O(16)-W(5)-O(15)#1	47.1(16)	C(13)-N(5)-C(17)	118(3)
O(2)-W(6)-O(12)	103.4(15)	C(13)-N(5)-Cu(2)	126(3)
O(2)-W(6)-O(14)	102.1(17)	C(17)-N(5)-Cu(2)	116(2)
O(12)-W(6)-O(14)	87.8(17)	C(18)-N(6)-N(7)	103(4)
O(2)-W(6)-O(22)	100.8(17)	C(19)-N(7)-N(6)	111(4)
O(12)-W(6)-O(22)	155.7(18)	C(20)-N(8)-C(24)	116(3)
O(14)-W(6)-O(22)	89.4(14)	C(20)-N(8)-Cu(1)	123(2)
O(2)-W(6)-O(19)	102.9(19)	C(24)-N(8)-Cu(1)	121(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1

Table S7 Anisotropic displacement parameters of compound **1**

	U11	U22	U33	U23	U13	U12
Si(1)	12(3)	17(2)	20(3)	-2(3)	-1(2)	1(3)
W(1)	38(1)	38(1)	28(1)	4(1)	2(1)	18(1)
W(2)	26(1)	36(1)	36(1)	4(1)	6(1)	-5(1)
W(3)	51(1)	29(1)	27(1)	0(1)	-8(1)	-1(1)
W(4)	44(1)	22(1)	34(1)	4(1)	14(1)	-7(1)
W(5)	35(1)	23(1)	55(1)	-13(1)	8(1)	5(1)
W(6)	36(1)	35(1)	36(1)	13(1)	18(1)	8(1)
O(1)	158(15)	33(7)	58(7)	9(6)	81(9)	17(8)
O(2)	83(11)	35(7)	59(7)	24(6)	-4(7)	-9(6)
O(3)	60(10)	29(6)	40(6)	-22(5)	1(6)	6(5)
O(4)	54(9)	67(7)	45(6)	19(6)	26(6)	27(7)
O(5)	145(15)	13(5)	63(7)	12(5)	67(9)	17(6)
O(6)	39(9)	61(7)	63(7)	21(6)	23(6)	13(6)
O(7)	158(16)	29(6)	80(8)	-6(6)	95(10)	5(8)
O(8)	77(11)	50(7)	29(6)	-11(5)	5(6)	0(6)
O(9)	96(12)	54(8)	31(6)	-10(5)	10(7)	25(7)
O(10)	88(12)	53(7)	34(6)	0(6)	-12(7)	38(7)
O(11)	37(10)	37(7)	171(12)	59(8)	-9(9)	-9(6)
O(12)	96(11)	46(7)	31(6)	0(5)	0(6)	46(7)
O(13)	43(10)	179(14)	48(7)	-55(8)	20(7)	-21(9)
O(14)	23(9)	175(13)	63(8)	-48(9)	15(7)	-18(9)
O(15)	37(9)	58(8)	100(9)	-18(7)	-2(8)	-2(6)
O(16)	52(10)	37(7)	144(11)	54(7)	-18(9)	6(7)
O(17)	51(11)	156(13)	46(7)	-31(8)	27(7)	-32(9)
O(18)	31(9)	48(8)	190(13)	52(9)	-7(10)	-3(6)
O(19)	42(8)	18(6)	39(6)	-1(4)	27(6)	9(4)
O(21)	41(14)	23(9)	17(9)	5(8)	18(9)	-2(10)
O(22)	25(13)	15(9)	24(10)	3(8)	-3(9)	0(8)
O(24)	49(10)	38(7)	81(8)	11(6)	40(8)	-3(6)
O(25)	106(13)	57(8)	40(7)	16(6)	40(8)	1(7)
O(26)	33(8)	36(6)	80(7)	-1(6)	19(6)	-2(6)
C(1)	44(13)	34(10)	63(11)	-5(8)	34(10)	7(8)
C(2)	38(12)	12(8)	82(13)	-9(8)	25(10)	10(7)
C(3)	36(12)	34(9)	27(8)	1(7)	5(8)	-6(8)
C(4)	130(20)	30(9)	31(9)	-1(8)	27(11)	-34(11)
C(5)	130(20)	41(11)	42(11)	-11(9)	10(13)	-16(12)
C(6)	110(20)	24(10)	136(18)	4(11)	100(17)	0(11)
C(7)	140(20)	6(8)	109(16)	3(9)	83(16)	-11(10)
C(8)	71(15)	16(8)	36(9)	-5(7)	29(9)	0(8)
C(9)	79(16)	37(10)	47(10)	2(9)	33(10)	13(10)
C(10)	100(20)	32(10)	69(13)	0(9)	26(13)	27(10)
C(11)	38(12)	25(9)	31(9)	5(7)	5(8)	-14(7)
C(12)	25(11)	45(10)	12(7)	-5(7)	-2(7)	-5(8)
C(13)	64(16)	58(12)	72(13)	-20(12)	32(12)	7(12)
C(14)	92(19)	37(11)	53(12)	-4(8)	25(12)	9(11)

C(15)	67(15)	16(8)	37(9)	0(7)	19(10)	-4(8)
C(16)	43(13)	36(10)	58(11)	-29(8)	32(10)	-10(8)
C(17)	74(17)	36(10)	45(10)	2(8)	19(11)	-19(10)
C(18)	41(14)	46(11)	57(12)	-2(9)	15(11)	-6(10)
Cu(1)	50(2)	25(1)	66(1)	-2(1)	25(1)	-1(1)
N(1)	65(12)	22(7)	51(9)	5(7)	17(8)	3(7)
N(2)	45(11)	27(8)	72(10)	-20(7)	24(9)	1(7)
N(3)	74(12)	20(7)	37(8)	-1(6)	24(8)	3(7)
N(4)	57(11)	31(8)	46(8)	1(6)	25(8)	-1(6)
N(5)	69(14)	43(9)	50(9)	-7(7)	36(9)	-10(9)

Table S8 Anisotropic displacement parameters of compound **2**

	U11	U22	U33	U23	U13	U12
Si(1)	42(7)	44(7)	23(6)	14(5)	-13(5)	-5(5)
W(1)	73(1)	23(1)	34(1)	8(1)	6(1)	-4(1)
W(2)	76(1)	60(1)	46(1)	33(1)	-38(1)	-34(1)
W(3)	48(1)	74(1)	31(1)	9(1)	-3(1)	-38(1)
W(4)	37(1)	70(1)	55(1)	46(1)	-4(1)	-9(1)
W(5)	39(1)	23(1)	39(1)	5(1)	5(1)	-8(1)
W(6)	48(1)	25(1)	39(1)	3(1)	-10(1)	-4(1)
Cu(1)	63(2)	29(2)	32(2)	9(1)	7(2)	1(2)
Cu(2)	41(2)	27(2)	33(2)	7(1)	2(2)	-1(1)
O(1)	82(16)	82(14)	65(14)	-29(11)	47(12)	-30(11)
O(2)	46(12)	71(12)	49(11)	35(9)	8(9)	10(9)
O(3)	26(10)	77(12)	62(12)	44(10)	10(9)	4(9)
O(4)	81(15)	47(11)	39(11)	9(8)	-1(10)	32(10)
O(6)	20(10)	71(12)	103(15)	57(11)	10(10)	23(9)
O(8)	37(11)	20(9)	61(12)	-6(8)	-20(9)	-8(7)
O(10)	105(17)	66(12)	23(10)	12(9)	8(10)	-30(11)
O(11)	62(14)	97(14)	31(11)	13(10)	8(10)	35(11)
O(12)	36(11)	47(10)	51(11)	22(8)	14(9)	31(8)
O(24)	44(11)	20(8)	18(9)	8(6)	2(8)	-3(7)
O(25)	59(12)	23(9)	33(10)	7(8)	-21(9)	-4(8)
C(2)	35(16)	30(14)	50(17)	23(12)	7(13)	9(11)
C(4)	100(20)	19(14)	27(15)	15(11)	-27(14)	2(14)
C(5)	70(20)	37(16)	34(16)	22(13)	12(15)	16(14)
C(6)	63(19)	25(14)	21(14)	-8(11)	2(13)	28(13)
C(10)	31(16)	53(18)	39(16)	10(13)	-19(12)	-13(13)
C(12)	45(19)	61(19)	80(20)	48(16)	-11(16)	-15(15)
C(14)	39(16)	15(12)	39(15)	-5(11)	-10(12)	19(11)
C(16)	11(13)	34(14)	36(15)	1(11)	12(11)	3(10)
C(17)	59(18)	12(12)	26(14)	4(10)	8(13)	-3(12)
C(22)	37(17)	70(19)	40(17)	34(15)	-26(13)	-23(14)
C(23)	37(18)	80(20)	37(18)	-7(15)	6(15)	14(15)
C(24)	35(19)	130(30)	60(20)	45(19)	-12(16)	-32(19)
C(27)	46(17)	16(13)	34(15)	4(11)	-25(12)	-17(11)

C(28)	31(15)	25(14)	34(15)	9(11)	-17(12)	-6(11)
C(29)	32(15)	31(14)	30(15)	18(12)	-5(12)	-4(11)
C(31)	52(18)	20(14)	62(19)	14(13)	-29(15)	-1(13)
C(33)	80(20)	27(15)	58(19)	16(14)	-18(16)	-16(14)
C(35)	38(17)	20(14)	56(18)	3(12)	6(14)	-11(12)
C(36)	61(19)	32(15)	14(13)	10(11)	-19(12)	-8(13)
N(2)	100(20)	20(12)	50(15)	18(10)	-21(13)	-13(11)
N(3)	24(12)	43(13)	7(10)	-2(9)	-9(9)	1(9)
N(4)	27(12)	32(11)	20(11)	11(9)	-7(9)	3(9)
N(7)	53(14)	17(10)	16(11)	-3(8)	-3(10)	1(9)
N(9)	49(14)	30(12)	21(11)	5(9)	-9(10)	-3(10)
N(10)	70(17)	29(13)	61(16)	9(11)	-13(13)	-24(11)
N(12)	34(12)	22(11)	28(12)	12(9)	-4(10)	-1(9)

Table S9 Anisotropic displacement parameters of compound **3**

	U11	U22	U33	U23	U13	U12
Si(1)	28(8)	43(9)	47(10)	33(8)	16(7)	18(7)
W(1)	30(1)	20(1)	20(1)	8(1)	19(1)	14(1)
W(2)	26(1)	19(1)	16(1)	7(1)	2(1)	4(1)
W(3)	26(1)	29(1)	14(1)	14(1)	12(1)	13(1)
W(4)	28(1)	25(1)	39(1)	23(1)	23(1)	6(1)
W(5)	19(1)	51(1)	29(1)	26(1)	15(1)	22(1)
W(6)	33(1)	30(1)	37(1)	29(1)	12(1)	15(1)
Cu(1)	45(3)	48(3)	38(3)	32(3)	21(2)	23(2)
Cu(2)	45(3)	43(3)	43(3)	33(3)	23(2)	24(2)
O(1)	51(17)	14(11)	48(16)	23(12)	41(14)	15(12)
O(2)	54(19)	33(15)	37(16)	29(14)	6(14)	10(14)
O(4)	26(15)	51(18)	100(30)	60(20)	26(16)	15(14)
O(5)	60(20)	21(13)	18(13)	10(11)	-7(13)	-6(13)
O(7)	45(19)	80(20)	170(40)	110(30)	70(20)	48(19)
O(8)	32(15)	62(19)	40(16)	30(15)	26(13)	37(15)
O(9)	45(18)	34(15)	38(17)	13(14)	14(14)	8(14)
O(11)	190(50)	60(20)	70(20)	60(20)	90(30)	90(30)
O(13)	180(50)	120(40)	60(20)	50(30)	70(30)	130(40)
O(14)	33(18)	70(20)	90(30)	10(20)	1(18)	37(18)
O(19)	60(20)	120(30)	28(18)	40(20)	-6(16)	-30(20)
O(21)	24(15)	70(20)	60(20)	51(19)	15(14)	-7(14)
O(22)	36(19)	44(19)	80(30)	-22(18)	-21(18)	30(16)
O(23)	40(15)	18(12)	29(13)	16(11)	24(12)	4(11)
O(24)	36(14)	26(13)	27(13)	25(11)	21(11)	15(11)
C(3)	13(18)	80(30)	70(30)	60(30)	13(19)	20(20)
C(8)	26(18)	18(16)	21(17)	13(14)	4(15)	6(14)
C(10)	30(20)	50(20)	60(30)	40(20)	20(20)	17(19)
C(11)	30(20)	50(30)	110(40)	70(30)	50(30)	30(20)
C(12)	30(20)	80(30)	30(20)	40(20)	11(18)	40(20)
C(13)	60(30)	70(30)	60(30)	60(30)	50(30)	60(30)

C(14)	30(20)	40(20)	50(20)	20(20)	21(19)	30(19)
C(17)	10(16)	40(20)	40(20)	30(19)	7(15)	1(15)
C(19)	40(20)	23(19)	50(30)	30(19)	30(20)	18(17)
C(20)	29(18)	11(14)	31(18)	16(14)	20(15)	14(14)
C(22)	30(20)	30(20)	60(30)	30(20)	10(20)	10(18)
C(23)	80(30)	50(30)	60(30)	40(20)	50(30)	50(30)
N(1)	28(17)	50(20)	35(18)	29(17)	15(15)	25(16)
N(2)	90(30)	33(19)	40(20)	26(18)	40(20)	30(20)
N(3)	50(20)	50(20)	50(20)	40(20)	30(20)	22(19)
N(6)	50(30)	50(20)	80(30)	40(20)	30(20)	40(20)
N(8)	25(16)	28(16)	23(16)	11(13)	7(13)	12(13)