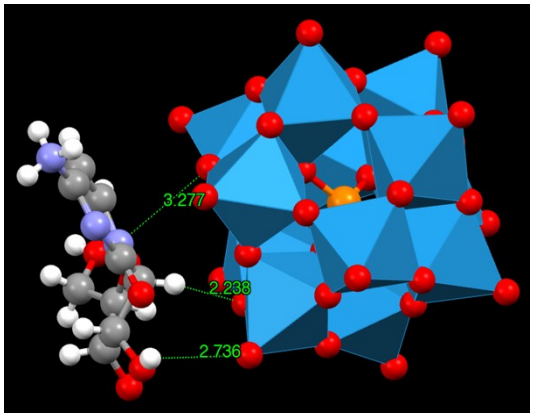
Supplementary Information

Molecular mechanisms behind potential genotoxicity of metal oxide nanoparticles: nucleoside deglycosylation pathway

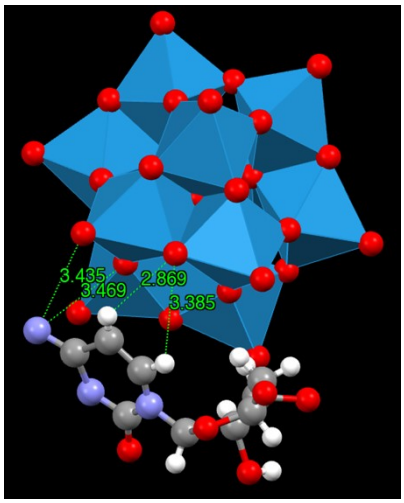
Fredric G. Svensson, Björn H. Greijer, Timothe Guerin, Tatiana Agback, Peter Agback, and Vadim G. Kessler*

Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala, Sweden

**Correspondence: vadim.kessler@slu.se*

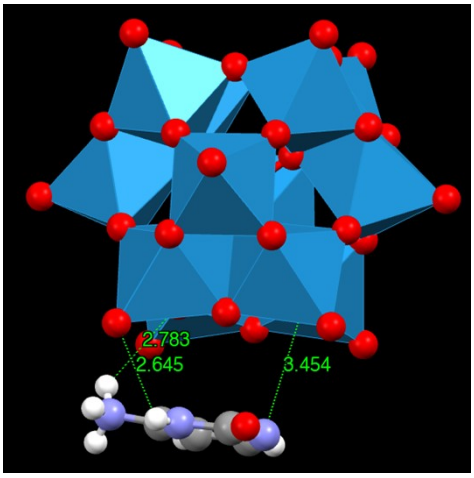


Supplementary Figure S1. Selected short contacts in compound **1**. N3C-O31 3.277 Å (terminal O), (C5C)H5CB-O32 2.238 Å (bridging O), (O2C)H2CB-O19 2.736 Å, (terminal O).

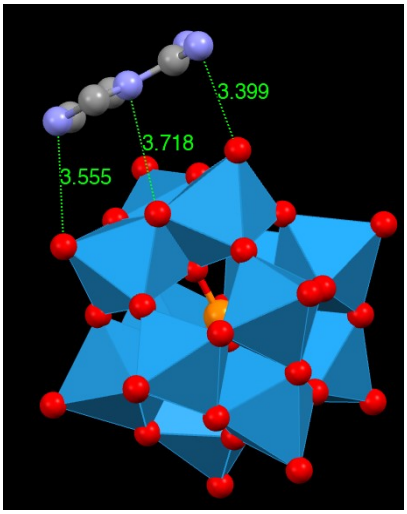


Supplementary Figure S2. Selected short contacts in compound **2**. N202-O35 3.435 Å (terminal O), N202-O48 3.469 Å (bridging O), (C209)H209-O21 2.869 Å (bridging O), (C208)H208-O21 3.385 Å (bridging O).

Supplementary Information

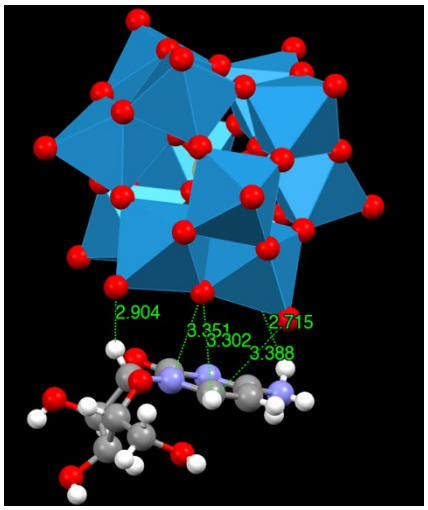


Supplementary Figure S3. Selected short contacts in compound **3**. (N1)H1B-O14 2.783 Å (bridging O), (N3)H3A-O1 2.645 Å (terminal O), N2-O9 3.454 Å (bridging O).

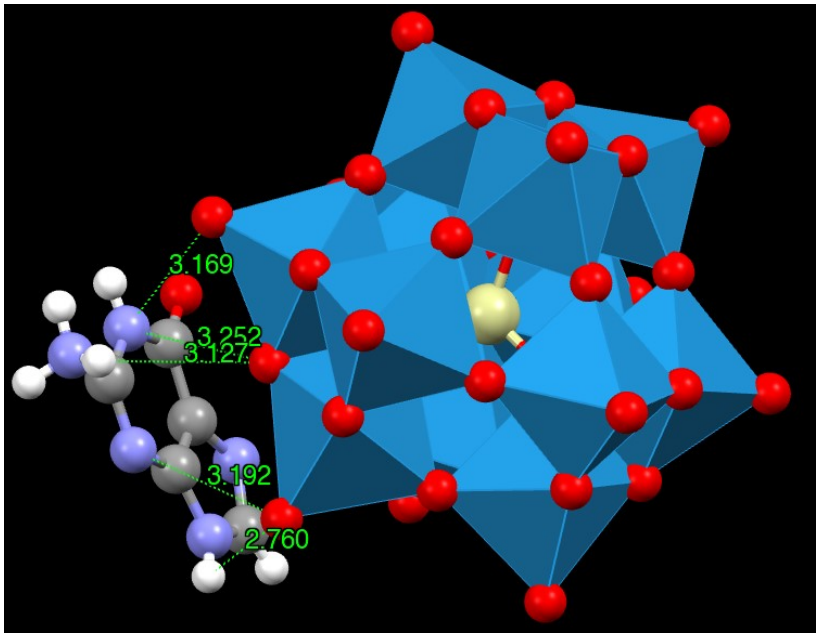


Supplementary Figure S4. Selected short contacts in compound **4.** N1A-O016 3.555 Å (terminal O), N2A-O00V 3.718 Å (bridging O), N3A-O01F 3.399 Å (terminal O). Hydrogen omitted due to the heavy disorder in the cytosine molecule.

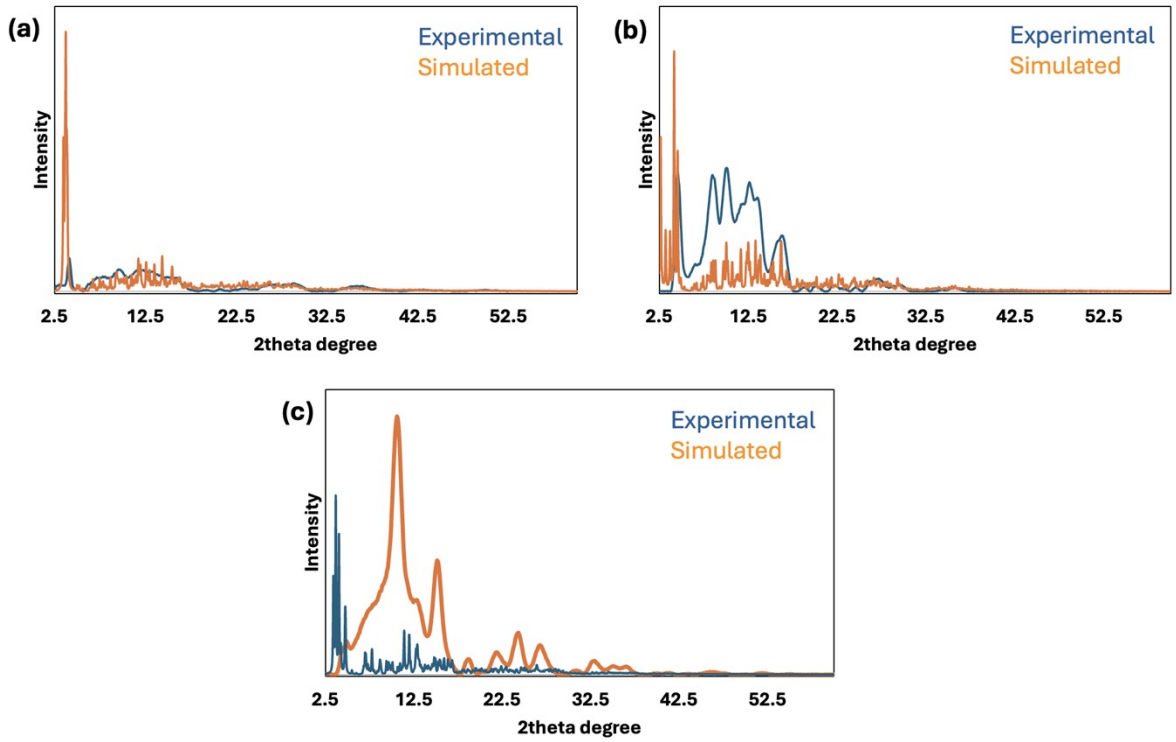
Supplementary Information



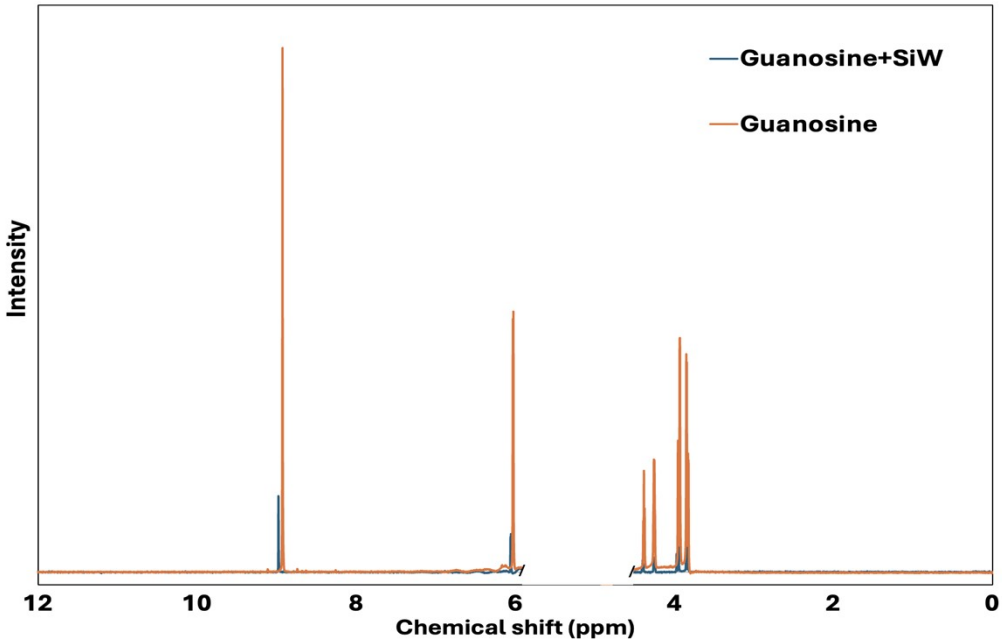
Supplementary Figure S5. Selected short contacts in compound **5**. (CF5)H5FA-O15A 2.904 Å (terminal O), N1F-O21A 3.351 Å (bridging O), (C4F)H4F4-O21A 3.302 Å (bridging O) (C4F)H4F4-O36A 3.338 Å (terminal O), N3F-H3F3-O22A 2.715 Å (terminal O).



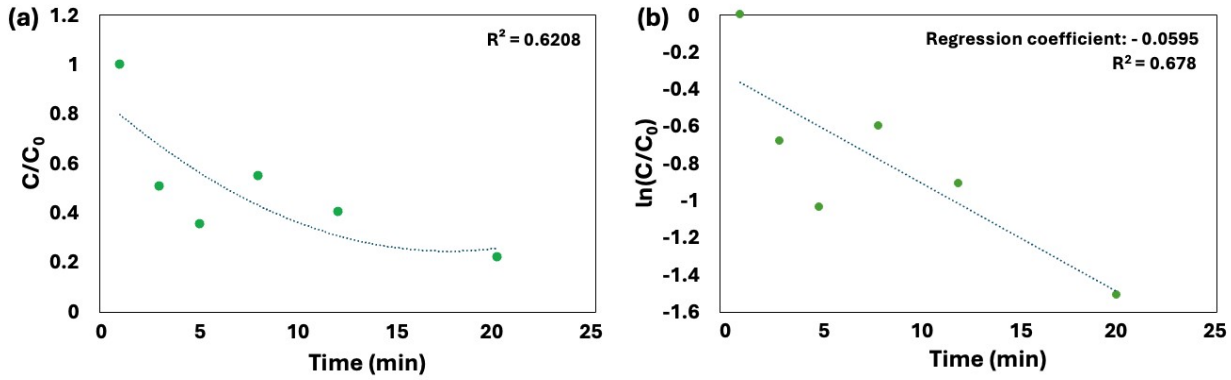
Supplementary Figure S6. Selected short contacts in compound **6.** N12-O38 3.169 Å (terminal O), N12-O22 3.252 Å (bridge O), N13-O2 3.192 Å (terminal O), (N14)H14A-O2 2.760 Å (terminal O), (N11)H11C-O22 3.127 Å (bridge O).



Supplementary Figure S7. Experimental and simulated powder XRD patterns for (a) compound **6**, (b) compound **2**, and (c) compound **4**.



Supplementary Figure S8. ^{1}H NMR spectrum of guanosine and guanosine with silicotungstic acid (1:1). The water signal (4.5 – 6 ppm) has been omitted for clarity.



Supplementary Figure S9. Kinetic plots of the deglycosylation of guanosine by phosphotungstate, (a) C/C_0 plot and (b) first-order plot.

Table S1. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for compound **1**.

x/a	y/b	z/c	U(eq)
W1	0.98295(5)	0.03380(5)	0.65686(3)	0.02029(16)
W2	0.54974(5)	0.96860(5)	0.60467(3)	0.02030(16)
W3	0.73354(6)	0.15848(5)	0.49419(2)	0.02062(16)
W4	0.74638(6)	0.93632(5)	0.53358(3)	0.02128(16)
W5	0.53463(5)	0.18987(5)	0.56309(3)	0.02051(16)
W6	0.76743(6)	0.06730(5)	0.73169(3)	0.02186(16)
W7	0.76699(6)	0.89204(5)	0.64767(3)	0.02215(16)
W8	0.96623(5)	0.07303(5)	0.54184(3)	0.01916(15)
W9	0.97161(6)	0.23742(5)	0.61659(3)	0.02055(16)
W10	0.55510(5)	0.14718(5)	0.68638(3)	0.02135(16)
W11	0.73482(6)	0.32009(5)	0.57203(3)	0.02192(16)
W12	0.76168(6)	0.27183(5)	0.69461(3)	0.02200(16)
P1	0.7566(3)	0.1072(2)	0.61197(14)	0.0089(7)
O39	0.0559(10)	0.3152(10)	0.6232(5)	0.031(3)
O1	0.0484(10)	0.0488(8)	0.5001(5)	0.023(3)

O2	0.7350(11)	0.1639(9)	0.4364(4)	0.028(3)
O3	0.7881(10)	0.1887(9)	0.7389(5)	0.027(3)
O4	0.0154(10)	0.1782(10)	0.5644(5)	0.030(3)
O5	0.7858(13)	0.7964(10)	0.6732(6)	0.038(4)
O6	0.7875(10)	0.0315(11)	0.7852(5)	0.031(3)
O7	0.5968(10)	0.3003(9)	0.5656(5)	0.026(3)
O8	0.5266(10)	0.0716(9)	0.5707(4)	0.023(3)
O9	0.7122(9)	0.0385(9)	0.5048(4)	0.021(3)
O10	0.7482(10)	0.2724(10)	0.5118(5)	0.032(3)
O11	0.0307(10)	0.1508(9)	0.6527(5)	0.024(3)
O12	0.7437(10)	0.9667(8)	0.6985(4)	0.021(3)
O13	0.0763(11)	0.9869(10)	0.6875(5)	0.030(3)
O14	0.7572(11)	0.8694(9)	0.4888(5)	0.027(3)
O15	0.8707(10)	0.2883(9)	0.5819(5)	0.025(3)
O16	0.4160(10)	0.2155(11)	0.5511(5)	0.034(4)
O17	0.0267(10)	0.0207(8)	0.5940(4)	0.021(3)
O18	0.7227(10)	0.3141(11)	0.6364(5)	0.031(3)
O19	0.4425(11)	0.1578(12)	0.7116(5)	0.037(4)
O20	0.5314(10)	0.1932(10)	0.6285(4)	0.026(3)
O21	0.8685(9)	0.1101(8)	0.6082(4)	0.019(3)
O22	0.7237(9)	0.1356(8)	0.6595(4)	0.018(3)
O23	0.8755(9)	0.9797(9)	0.5380(5)	0.024(3)
O24	0.7425(12)	0.4237(9)	0.5612(5)	0.033(3)
O25	0.6114(9)	0.9230(10)	0.5507(5)	0.026(3)
O26	0.5421(10)	0.0398(9)	0.6574(4)	0.025(3)
O27	0.8937(10)	0.9408(10)	0.6459(5)	0.028(3)
O28	0.8960(10)	0.0646(9)	0.7051(4)	0.021(3)

O29	0.6242(10)	0.2468(10)	0.7043(5)	0.027(3)
O30	0.7800(11)	0.3580(11)	0.7260(5)	0.034(4)
O31	0.6266(9)	0.8898(9)	0.6395(4)	0.022(3)
O32	0.6309(9)	0.0904(9)	0.7337(4)	0.022(3)
O33	0.7777(10)	0.8645(9)	0.5850(5)	0.027(3)
O34	0.8674(9)	0.1353(10)	0.5106(5)	0.026(3)
O35	0.7110(9)	0.1672(9)	0.5766(4)	0.020(3)
O36	0.5947(10)	0.1740(9)	0.5053(5)	0.024(3)
O37	0.4379(10)	0.9194(10)	0.6043(5)	0.030(3)
O38	0.7207(9)	0.0158(9)	0.6027(5)	0.022(3)
O40	0.8889(9)	0.2558(9)	0.6679(5)	0.022(3)
N2B	0.7395(12)	0.5171(12)	0.3743(5)	0.026(4)
O1A	0.7807(12)	0.6343(11)	0.7703(6)	0.040(4)
O5C	0.7435(15)	0.8348(14)	0.8422(6)	0.060(6)
O1B	0.6854(12)	0.6511(10)	0.3713(5)	0.032(3)
O1C	0.3437(13)	0.9467(12)	0.7072(6)	0.043(4)
N3A	0.9159(14)	0.6554(12)	0.7275(6)	0.030(4)
O4C	0.5968(15)	0.8889(15)	0.7774(7)	0.059(6)
N3B	0.7060(13)	0.5931(11)	0.4415(6)	0.027(4)
O4A	0.9920(13)	0.5470(11)	0.6860(6)	0.041(4)
N3C	0.4749(17)	0.8577(13)	0.7250(6)	0.039(5)
O3B	0.4445(12)	0.7236(13)	0.5213(7)	0.052(5)
N2C	0.3428(16)	0.8083(14)	0.6814(8)	0.044(5)
O2A	0.7799(17)	0.5071(12)	0.6535(6)	0.056(5)
C1A	0.8456(17)	0.6800(14)	0.7584(7)	0.029(5)
C2B	0.7628(15)	0.4463(16)	0.3977(8)	0.036(5)
N1B	0.7865(15)	0.3816(13)	0.3740(8)	0.042(5)

O3C	0.5190(19)	0.0328(14)	0.8584(8)	0.070(7)
C4B	0.7340(16)	0.5229(14)	0.4660(8)	0.032(5)
N2A	0.8580(14)	0.7629(12)	0.7745(7)	0.033(4)
O2B	0.5393(16)	0.7657(15)	0.4443(7)	0.066(6)
O4B	0.6970(13)	0.6698(12)	0.5082(6)	0.046(5)
C6B	0.5564(16)	0.6836(15)	0.4595(8)	0.033(5)
C8B	0.6180(18)	0.7014(15)	0.5338(8)	0.035(5)
C3B	0.7631(15)	0.4519(13)	0.4450(7)	0.027(4)
O5A	0.1212(15)	0.6470(14)	0.6277(7)	0.057(6)
C7A	0.904(2)	0.6027(14)	0.6238(7)	0.035(5)
O5B	0.626(2)	0.5868(15)	0.5885(8)	0.077(8)
C4C	0.5250(19)	0.7818(13)	0.7163(8)	0.036(5)
C3C	0.4835(18)	0.7205(14)	0.6913(8)	0.037(5)
C4A	0.9932(17)	0.709(2)	0.7144(9)	0.050(8)
C8A	0.990(2)	0.5436(15)	0.6363(8)	0.038(6)
O3A	0.8645(17)	0.5853(17)	0.5803(7)	0.067(7)
C1C	0.3861(19)	0.8782(19)	0.7055(8)	0.042(6)
C2A	0.9279(19)	0.8181(18)	0.7622(9)	0.044(7)
C5C	0.5137(19)	0.9263(18)	0.7551(7)	0.042(6)
O2C	0.3964(16)	0.0304(15)	0.7896(8)	0.067(6)
C1B	0.7066(15)	0.5913(17)	0.3937(7)	0.035(6)
C5A	0.9005(18)	0.5723(14)	0.7034(8)	0.033(5)
C2C	0.387(2)	0.7319(16)	0.6763(9)	0.042(6)
N1A	0.929(2)	0.8920(15)	0.7800(8)	0.062(8)
C7C	0.5040(18)	0.9561(19)	0.8375(9)	0.044(6)
C6C	0.4451(19)	0.9510(17)	0.7956(9)	0.045(6)
C9A	0.094(2)	0.561(2)	0.6171(10)	0.058(8)

C8C	0.606(2)	0.9186(18)	0.8237(9)	0.043(6)
C6A	0.8317(19)	0.5856(18)	0.6634(8)	0.044(6)
N1C	0.3374(18)	0.6727(18)	0.6535(8)	0.060(7)
C3A	0.002(2)	0.7853(18)	0.7311(9)	0.048(7)
C9C	0.644(2)	0.852(3)	0.8533(11)	0.077(12)
C9B	0.636(2)	0.6758(17)	0.5839(8)	0.048(7)
C7B	0.5241(18)	0.6752(17)	0.5095(9)	0.042(6)
C5B	0.6705(19)	0.6722(18)	0.4617(8)	0.043(6)

Table S2. Bond lengths (Å) for compound **1**.

W1-O13	1.718(14)	W1-O28	1.901(13)
W1-O27	1.928(15)	W1-O17	1.944(13)
W1-O11	1.960(14)	W1-O21	2.424(13)
W2-O37	1.702(14)	W2-O26	1.911(13)
W2-O31	1.915(13)	W2-O25	1.925(14)
W2-O8	1.931(13)	W2-O38	2.432(12)
W3-O2	1.694(13)	W3-O10	1.881(16)
W3-O34	1.910(13)	W3-O36	1.923(14)
W3-O9	1.940(14)	W3-O35	2.434(12)
W4-O14	1.690(13)	W4-O9	1.877(14)
W4-O23	1.882(13)	W4-O25	1.907(13)
W4-O33	1.931(14)	W4-O38	2.406(13)
W5-O16	1.693(13)	W5-O8	1.881(13)
W5-O36	1.894(14)	W5-O20	1.915(13)
W5-O7	1.936(15)	W5-O35	2.447(12)
W6-O6	1.687(14)	W6-O12	1.888(13)
W6-O32	1.886(13)	W6-O28	1.908(13)

W6-O3	1.946(15)	W6-O22	2.446(12)
W7-O5	1.702(15)	W7-O27	1.881(14)
W7-O33	1.890(15)	W7-O31	1.916(12)
W7-O12	1.924(13)	W7-O38	2.436(14)
W8-O1	1.695(13)	W8-O34	1.896(14)
W8-O4	1.906(16)	W8-O23	1.922(14)
W8-O17	1.920(13)	W8-O21	2.423(13)
W9-O39	1.687(15)	W9-O15	1.882(14)
W9-O4	1.886(16)	W9-O40	1.896(13)
W9-O11	1.904(13)	W9-O21	2.458(12)
W10-O19	1.702(14)	W10-O20	1.872(14)
W10-O26	1.903(14)	W10-O29	1.904(15)
W10-O32	1.943(13)	W10-O22	2.422(12)
W11-O24	1.669(14)	W11-O18	1.893(14)
W11-O7	1.905(14)	W11-O15	1.929(14)
W11-O10	1.925(16)	W11-O35	2.437(14)
W12-O30	1.659(16)	W12-O3	1.878(14)
W12-O18	1.905(15)	W12-O40	1.909(13)
W12-O29	1.924(14)	W12-O22	2.437(13)
P1-O21	1.521(13)	P1-O22	1.527(12)
P1-O35	1.533(13)	P1-O38	1.545(14)
N2B-C2B	1.35(3)	N2B-C1B	1.37(3)
O1A-C1A	1.19(3)	O5C-C9C	1.42(3)
O1B-C1B	1.18(3)	O1C-C1C	1.22(3)
N3A-C1A	1.37(3)	N3A-C4A	1.39(3)
N3A-C5A	1.50(3)	O4C-C5C	1.43(3)
O4C-C8C	1.44(3)	N3B-C4B	1.37(3)

N3B-C1B	1.40(3)	N3B-C5B	1.46(3)
O4A-C5A	1.40(3)	O4A-C8A	1.46(3)
N3C-C1C	1.37(3)	N3C-C4C	1.40(3)
N3C-C5C	1.49(3)	O3B-C7B	1.37(3)
N2C-C2C	1.36(3)	N2C-C1C	1.43(4)
O2A-C6A	1.45(3)	C1A-N2A	1.40(3)
C2B-N1B	1.27(3)	C2B-C3B	1.39(3)
O3C-C7C	1.37(3)	C4B-C3B	1.34(3)
N2A-C2A	1.34(4)	O2B-C6B	1.39(3)
O4B-C8B	1.40(3)	O4B-C5B	1.41(3)
C6B-C7B	1.53(3)	C6B-C5B	1.56(3)
C8B-C7B	1.52(3)	C8B-C9B	1.54(3)
O5A-C9A	1.43(4)	C7A-O3A	1.41(3)
C7A-C8A	1.54(3)	C7A-C6A	1.54(3)
O5B-C9B	1.42(3)	C4C-C3C	1.34(3)
C3C-C2C	1.39(4)	C4A-C3A	1.31(4)
C8A-C9A	1.53(4)	C2A-N1A	1.28(3)
C2A-C3A	1.45(4)	C5C-C6C	1.56(4)
O2C-C6C	1.43(3)	C5A-C6A	1.51(3)
C2C-N1C	1.33(4)	C7C-C6C	1.46(4)
C7C-C8C	1.55(3)	C8C-C9C	1.46(4)

Table S3. Bond angles (°) for compound **1**.

O13-W1-O28	100.2(7)	O13-W1-O27	102.8(7)
O28-W1-O27	86.0(6)	O13-W1-O17	103.0(7)

Supplementary Information

O28-W1-O17	156.7(6)	O27-W1-O17	87.3(6)
O13-W1-O11	101.2(6)	O28-W1-O11	90.6(6)
O27-W1-O11	156.0(6)	O17-W1-O11	86.6(6)
O13-W1-O21	172.3(6)	O28-W1-O21	85.0(5)
O27-W1-O21	83.1(5)	O17-W1-O21	72.1(5)
O11-W1-O21	73.0(5)	O37-W2-O26	102.9(7)
O37-W2-O31	101.0(6)	O26-W2-O31	88.9(6)
O37-W2-O25	102.2(7)	O26-W2-O25	154.8(6)
O31-W2-O25	87.6(6)	O37-W2-O8	103.6(7)
O26-W2-O8	85.0(6)	O31-W2-O8	155.3(5)
O25-W2-O8	87.9(6)	O37-W2-O38	170.6(6)
O26-W2-O38	83.7(5)	O31-W2-O38	72.2(5)
O25-W2-O38	71.5(5)	O8-W2-O38	83.4(5)
O2-W3-O10	103.0(6)	O2-W3-O34	104.4(6)
O10-W3-O34	90.8(7)	O2-W3-O36	100.0(6)
O10-W3-O36	86.3(6)	O34-W3-O36	155.5(6)
O2-W3-O9	102.1(6)	O10-W3-O9	154.8(6)
O34-W3-O9	85.1(6)	O36-W3-O9	87.2(6)
O2-W3-O35	171.0(6)	O10-W3-O35	71.8(5)
O34-W3-O35	83.2(5)	O36-W3-O35	72.7(5)
O9-W3-O35	83.0(5)	O14-W4-O9	102.0(6)
O14-W4-O23	101.5(6)	O9-W4-O23	87.0(6)
O14-W4-O25	102.6(6)	O9-W4-O25	88.6(6)
O23-W4-O25	155.9(6)	O14-W4-O33	102.7(6)
O9-W4-O33	155.3(6)	O23-W4-O33	87.5(6)
O25-W4-O33	86.6(6)	O14-W4-O38	172.2(6)
O9-W4-O38	84.0(5)	O23-W4-O38	83.6(5)

Supplementary Information

O25-W4-O38	72.4(5)	O33-W4-O38	71.4(5)
O16-W5-O8	101.9(7)	O16-W5-O36	104.7(7)
O8-W5-O36	90.0(6)	O16-W5-O20	100.3(7)
O8-W5-O20	84.7(6)	O36-W5-O20	155.0(6)
O16-W5-O7	101.9(7)	O8-W5-O7	155.9(6)
O36-W5-O7	88.1(6)	O20-W5-O7	87.0(6)
O16-W5-O35	173.9(7)	O8-W5-O35	83.8(5)
O36-W5-O35	72.9(5)	O20-W5-O35	82.2(5)
O7-W5-O35	72.6(5)	O6-W6-O12	102.9(7)
O6-W6-O32	101.2(6)	O12-W6-O32	90.7(6)
O6-W6-O28	103.0(6)	O12-W6-O28	85.8(6)
O32-W6-O28	155.8(6)	O6-W6-O3	101.9(7)
O12-W6-O3	155.1(5)	O32-W6-O3	87.0(6)
O28-W6-O3	86.3(6)	O6-W6-O22	171.5(6)
O12-W6-O22	83.4(5)	O32-W6-O22	72.8(5)
O28-W6-O22	83.0(5)	O3-W6-O22	72.2(5)
O5-W7-O27	103.7(7)	O5-W7-O33	102.1(7)
O27-W7-O33	89.8(6)	O5-W7-O31	100.8(7)
O27-W7-O31	155.4(6)	O33-W7-O31	87.2(6)
O5-W7-O12	103.2(7)	O27-W7-O12	85.5(6)
O33-W7-O12	154.7(5)	O31-W7-O12	86.9(6)
O5-W7-O38	170.2(6)	O27-W7-O38	83.8(5)
O33-W7-O38	71.3(5)	O31-W7-O38	72.1(5)
O12-W7-O38	83.4(5)	O1-W8-O34	103.4(6)
O1-W8-O4	102.5(6)	O34-W8-O4	87.9(6)
O1-W8-O23	101.8(6)	O34-W8-O23	85.3(6)
O4-W8-O23	155.7(6)	O1-W8-O17	101.3(6)

Supplementary Information

O34-W8-O17	155.3(6)	O4-W8-O17	87.1(6)
O23-W8-O17	89.5(6)	O1-W8-O21	172.1(5)
O34-W8-O21	82.9(5)	O4-W8-O21	72.7(5)
O23-W8-O21	83.3(5)	O17-W8-O21	72.5(5)
O39-W9-O15	104.1(7)	O39-W9-O4	103.9(7)
O15-W9-O4	90.2(6)	O39-W9-O40	101.3(6)
O15-W9-O40	86.2(6)	O4-W9-O40	154.6(6)
O39-W9-O11	100.0(7)	O15-W9-O11	155.6(6)
O4-W9-O11	87.8(6)	O40-W9-O11	85.3(6)
O39-W9-O21	171.9(6)	O15-W9-O21	83.2(5)
O4-W9-O21	72.2(6)	O40-W9-O21	82.5(5)
O11-W9-O21	73.0(5)	O19-W10-O20	101.6(7)
O19-W10-O26	101.4(8)	O20-W10-O26	85.7(6)
O19-W10-O29	103.9(7)	O20-W10-O29	90.8(6)
O26-W10-O29	154.7(6)	O19-W10-O32	102.1(6)
O20-W10-O32	156.2(6)	O26-W10-O32	87.5(6)
O29-W10-O32	85.7(6)	O19-W10-O22	173.1(6)
O20-W10-O22	84.0(5)	O26-W10-O22	82.8(5)
O29-W10-O22	71.8(5)	O32-W10-O22	72.5(5)
O24-W11-O18	104.1(7)	O24-W11-O7	101.7(7)
O18-W11-O7	90.3(6)	O24-W11-O15	102.9(7)
O18-W11-O15	85.4(6)	O7-W11-O15	155.3(6)
O24-W11-O10	101.7(7)	O18-W11-O10	154.1(7)
O7-W11-O10	86.5(6)	O15-W11-O10	86.9(6)
O24-W11-O35	171.2(6)	O18-W11-O35	83.4(6)
O7-W11-O35	73.3(5)	O15-W11-O35	82.0(5)
O10-W11-O35	71.1(5)	O30-W12-O3	99.3(7)

O30-W12-O18	104.5(8)	O3-W12-O18	156.2(7)
O30-W12-O40	101.5(7)	O3-W12-O40	91.0(6)
O18-W12-O40	86.0(6)	O30-W12-O29	103.3(7)
O3-W12-O29	86.5(6)	O18-W12-O29	86.3(6)
O40-W12-O29	155.1(6)	O30-W12-O22	170.9(6)
O3-W12-O22	73.5(5)	O18-W12-O22	82.7(6)
O40-W12-O22	84.3(5)	O29-W12-O22	71.2(5)
O21-P1-O22	110.3(7)	O21-P1-O35	109.5(7)
O22-P1-O35	108.4(7)	O21-P1-O38	109.2(7)
O22-P1-O38	110.0(7)	O35-P1-O38	109.3(8)
W12-O3-W6	125.8(7)	W9-O4-W8	127.0(8)
W11-O7-W5	125.3(7)	W5-O8-W2	152.4(8)
W4-O9-W3	150.8(7)	W3-O10-W11	127.9(7)
W9-O11-W1	124.8(7)	W6-O12-W7	152.2(7)
W9-O15-W11	152.2(8)	W8-O17-W1	125.2(7)
W11-O18-W12	152.1(9)	W10-O20-W5	152.9(9)
P1-O21-W8	126.5(7)	P1-O21-W1	125.5(7)
W8-O21-W1	90.1(4)	P1-O21-W9	125.7(8)
W8-O21-W9	88.1(4)	W1-O21-W9	89.1(4)
P1-O22-W10	126.4(7)	P1-O22-W12	125.6(7)
W10-O22-W12	89.7(4)	P1-O22-W6	125.9(7)
W10-O22-W6	88.9(4)	W12-O22-W6	88.4(4)
W4-O23-W8	151.2(8)	W4-O25-W2	126.2(7)
W10-O26-W2	151.4(8)	W7-O27-W1	151.4(8)
W6-O28-W1	150.9(7)	W10-O29-W12	127.2(8)
W7-O31-W2	126.4(7)	W6-O32-W10	125.8(7)
W7-O33-W4	127.2(7)	W8-O34-W3	152.9(8)

Supplementary Information

P1-O35-W3	125.7(8)	P1-O35-W5	126.3(7)
W3-O35-W5	88.3(4)	P1-O35-W11	126.5(7)
W3-O35-W11	89.1(4)	W5-O35-W11	88.6(4)
W5-O36-W3	126.0(7)	P1-O38-W4	126.0(7)
P1-O38-W7	124.9(7)	W4-O38-W7	90.0(5)
P1-O38-W2	125.5(7)	W4-O38-W2	89.9(4)
W7-O38-W2	89.3(4)	W9-O40-W12	151.3(8)
C2B-N2B-C1B	124.9(17)	C1A-N3A-C4A	122.(2)
C1A-N3A-C5A	117.4(19)	C4A-N3A-C5A	120.(2)
C5C-O4C-C8C	111.(2)	C4B-N3B-C1B	120.(2)
C4B-N3B-C5B	124.6(19)	C1B-N3B-C5B	115.(2)
C5A-O4A-C8A	111.0(18)	C1C-N3C-C4C	124.(2)
C1C-N3C-C5C	113.(2)	C4C-N3C-C5C	124.(2)
C2C-N2C-C1C	124.(2)	O1A-C1A-N3A	122.(2)
O1A-C1A-N2A	124.(2)	N3A-C1A-N2A	114.(2)
N1B-C2B-N2B	116.(2)	N1B-C2B-C3B	126.(2)
N2B-C2B-C3B	117.(2)	C3B-C4B-N3B	121.(2)
C2A-N2A-C1A	127.(2)	C8B-O4B-C5B	108.3(19)
O2B-C6B-C7B	110.(2)	O2B-C6B-C5B	107.(2)
C7B-C6B-C5B	104.(2)	O4B-C8B-C7B	107.0(19)
O4B-C8B-C9B	107.(2)	C7B-C8B-C9B	121.(2)
C4B-C3B-C2B	121.(2)	O3A-C7A-C8A	113.(2)
O3A-C7A-C6A	114.(2)	C8A-C7A-C6A	101.5(18)
C3C-C4C-N3C	121.(2)	C4C-C3C-C2C	118.(2)
C3A-C4A-N3A	121.(3)	O4A-C8A-C7A	103.1(19)
O4A-C8A-C9A	110.(2)	C7A-C8A-C9A	120.(2)
O1C-C1C-N3C	127.(3)	O1C-C1C-N2C	120.(2)

N3C-C1C-N2C	112.(2)	N1A-C2A-N2A	120.(3)
N1A-C2A-C3A	125.(3)	N2A-C2A-C3A	115.(2)
O4C-C5C-N3C	104.(2)	O4C-C5C-C6C	103.0(18)
N3C-C5C-C6C	115.(2)	O1B-C1B-N2B	122.(2)
O1B-C1B-N3B	122.(2)	N2B-C1B-N3B	116.(2)
O4A-C5A-N3A	107.2(19)	O4A-C5A-C6A	108.(2)
N3A-C5A-C6A	109.1(19)	N2C-C2C-N1C	117.(3)
N2C-C2C-C3C	120.(2)	N1C-C2C-C3C	123.(3)
O3C-C7C-C6C	120.(3)	O3C-C7C-C8C	109.(2)
C6C-C7C-C8C	104.(2)	C7C-C6C-O2C	108.(2)
C7C-C6C-C5C	109.(2)	O2C-C6C-C5C	114.(2)
O5A-C9A-C8A	109.(2)	C9C-C8C-O4C	111.(3)
C9C-C8C-C7C	116.(2)	O4C-C8C-C7C	107.(2)
O2A-C6A-C5A	110.(2)	O2A-C6A-C7A	107.8(19)
C5A-C6A-C7A	103.(2)	C4A-C3A-C2A	120.(3)
O5C-C9C-C8C	110.(2)	O5B-C9B-C8B	110.(2)
O3B-C7B-C8B	113.(2)	O3B-C7B-C6B	115.(2)
C8B-C7B-C6B	100.7(19)	O4B-C5B-N3B	106.(2)
O4B-C5B-C6B	107.(2)	N3B-C5B-C6B	114.(2)

Table S4. Anisotropic atomic displacement parameters (Å2) for compound **1**.

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W1	0.0127(3)	0.0277(4)	0.0205(4)	0.0027(3)	-0.0010(3)	0.0017(3)
W2	0.0141(3)	0.0231(4)	0.0237(4)	0.0027(3)	0.0005(3)	-0.0033(3)

W3	0.0183(3)	0.0274(4)	0.0162(3)	0.0040(3)	-0.0013(3)	-0.0018(3)
W4	0.0184(4)	0.0228(4)	0.0227(4)	-0.0028(3)	0.0010(3)	-0.0026(3)
W5	0.0139(3)	0.0262(4)	0.0214(4)	0.0044(3)	-0.0024(3)	0.0016(3)
W6	0.0165(3)	0.0328(4)	0.0163(3)	0.0027(3)	0.0000(3)	0.0013(3)
W7	0.0204(4)	0.0203(4)	0.0258(4)	0.0053(3)	-0.0031(3)	-0.0009(3)
W8	0.0129(3)	0.0248(4)	0.0198(4)	-0.0001(3)	0.0019(3)	-0.0006(3)
W9	0.0138(3)	0.0240(4)	0.0238(4)	0.0002(3)	-0.0009(3)	-0.0041(3)
W10	0.0143(3)	0.0303(4)	0.0195(4)	0.0015(3)	0.0022(3)	0.0014(3)
W11	0.0219(4)	0.0200(4)	0.0238(4)	0.0038(3)	-0.0035(3)	-0.0017(3)
W12	0.0197(4)	0.0256(4)	0.0207(4)	-0.0039(3)	-0.0002(3)	-0.0001(3)
P1	0.0114(18)	0.0057(16)	0.0096(17)	0.0003(13)	0.0014(14)	0.0010(14)
O39	0.019(7)	0.049(10)	0.025(7)	-0.009(7)	0.003(6)	-0.010(7)
O1	0.018(6)	0.021(7)	0.030(7)	-0.008(5)	0.004(6)	-0.007(5)
O2	0.029(7)	0.038(8)	0.017(6)	0.007(6)	0.002(6)	-0.002(7)
O3	0.029(8)	0.028(8)	0.023(7)	0.001(6)	-0.005(6)	-0.006(6)
O4	0.017(7)	0.047(9)	0.026(7)	0.007(7)	-0.007(6)	0.000(6)
O5	0.045(10)	0.025(8)	0.043(9)	0.010(7)	-0.009(7)	-0.004(7)
O6	0.023(7)	0.046(9)	0.024(7)	0.013(7)	0.001(6)	0.000(7)
O7	0.021(7)	0.028(8)	0.027(8)	0.000(6)	0.002(6)	0.002(6)
O8	0.025(7)	0.023(7)	0.020(6)	0.008(5)	-0.007(5)	-0.006(6)
O9	0.016(6)	0.027(7)	0.019(6)	0.001(6)	-0.002(5)	0.000(5)
O10	0.022(7)	0.040(8)	0.032(8)	0.022(7)	0.002(6)	-0.013(7)
O11	0.022(7)	0.026(7)	0.023(7)	0.006(6)	-0.010(6)	-0.006(6)
O12	0.022(7)	0.016(6)	0.024(6)	0.009(5)	-0.004(5)	-0.006(6)
O13	0.025(7)	0.032(8)	0.032(8)	0.002(7)	-0.009(6)	0.001(6)
O14	0.026(7)	0.030(7)	0.024(7)	-0.006(6)	-0.002(6)	0.001(6)
O15	0.019(7)	0.031(8)	0.026(7)	-0.002(6)	-0.001(6)	0.000(6)

O16	0.014(7)	0.051(10)	0.037(9)	0.007(8)	-0.010(6)	0.004(7)
O17	0.020(3)	0.021(3)	0.021(3)	0.0004(14)	-0.0003(14)	0.0008(14)
O18	0.018(7)	0.049(10)	0.025(7)	0.000(7)	0.003(6)	0.001(7)
O19	0.019(7)	0.063(11)	0.030(8)	-0.002(8)	0.007(6)	0.014(7)
O20	0.020(7)	0.036(8)	0.020(7)	-0.005(6)	-0.002(5)	-0.001(6)
O21	0.013(6)	0.021(7)	0.023(7)	0.006(5)	-0.001(5)	-0.010(5)
O22	0.020(6)	0.026(7)	0.010(5)	0.004(5)	0.006(5)	-0.001(5)
O23	0.018(6)	0.033(8)	0.019(7)	0.004(6)	0.008(5)	0.002(6)
O24	0.038(9)	0.021(7)	0.039(8)	0.000(6)	0.000(7)	0.006(7)
O25	0.014(6)	0.032(8)	0.031(8)	-0.008(6)	-0.004(5)	-0.002(6)
O26	0.024(7)	0.035(8)	0.015(6)	-0.004(6)	-0.003(5)	0.005(6)
O27	0.020(7)	0.034(9)	0.030(8)	0.000(7)	-0.003(6)	0.004(6)
O28	0.021(6)	0.029(8)	0.014(6)	-0.007(6)	0.000(5)	0.003(6)
O29	0.020(7)	0.036(9)	0.025(8)	-0.006(6)	0.000(6)	0.004(6)
O30	0.026(8)	0.046(10)	0.029(8)	-0.011(7)	-0.005(6)	0.006(7)
O31	0.012(6)	0.033(8)	0.022(7)	0.013(6)	0.001(5)	-0.005(5)
O32	0.016(6)	0.033(8)	0.017(6)	0.007(6)	0.004(5)	-0.001(5)
O33	0.021(7)	0.024(7)	0.036(8)	0.000(6)	-0.005(6)	0.007(6)
O34	0.011(6)	0.044(9)	0.021(7)	0.004(6)	0.001(5)	-0.006(6)
O35	0.015(6)	0.037(8)	0.009(6)	0.003(5)	-0.004(5)	-0.001(5)
O36	0.020(7)	0.032(8)	0.020(7)	0.002(6)	-0.002(5)	-0.009(6)
O37	0.011(6)	0.047(9)	0.032(8)	0.003(7)	-0.001(6)	-0.001(6)
O38	0.011(6)	0.028(7)	0.027(7)	-0.002(6)	0.001(5)	-0.002(5)
O40	0.014(6)	0.029(8)	0.024(7)	-0.006(6)	-0.002(5)	0.002(5)
N2B	0.016(8)	0.043(10)	0.021(8)	0.006(7)	0.001(6)	-0.007(7)
O1A	0.036(9)	0.039(9)	0.046(10)	0.005(8)	0.004(8)	-0.002(8)
O5C	0.055(12)	0.085(15)	0.040(10)	-0.003(10)	-0.011(9)	0.037(12)

O1B	0.046(9)	0.029(8)	0.022(7)	0.010(6)	0.007(6)	0.007(7)
O1C	0.038(9)	0.057(12)	0.034(9)	0.007(8)	-0.005(7)	0.003(9)
N3A	0.033(10)	0.026(9)	0.029(9)	-0.006(8)	-0.003(8)	0.001(8)
O4C	0.044(11)	0.086(16)	0.047(12)	-0.002(11)	-0.003(9)	0.006(11)
N3B	0.030(9)	0.028(9)	0.024(9)	-0.002(7)	0.006(7)	-0.006(7)
O4A	0.041(9)	0.040(10)	0.044(10)	0.002(8)	0.003(8)	0.024(8)
N3C	0.054(13)	0.032(10)	0.029(10)	0.001(8)	-0.005(9)	-0.003(10)
O3B	0.028(9)	0.069(13)	0.058(12)	-0.014(10)	0.011(8)	-0.006(9)
N2C	0.042(12)	0.039(12)	0.050(13)	0.002(10)	0.008(10)	0.003(10)
O2A	0.081(15)	0.051(12)	0.036(10)	-0.005(9)	-0.011(10)	-0.017(11)
C1A	0.034(11)	0.029(11)	0.024(10)	0.003(9)	-0.007(9)	0.010(9)
C2B	0.014(9)	0.054(15)	0.039(12)	-0.012(11)	0.008(9)	0.012(10)
N1B	0.034(11)	0.039(12)	0.054(13)	0.003(10)	-0.012(9)	0.000(9)
O3C	0.088(17)	0.054(13)	0.070(15)	-0.032(11)	-0.013(13)	0.013(12)
C4B	0.029(10)	0.033(11)	0.033(11)	0.006(9)	0.004(9)	0.010(9)
N2A	0.038(10)	0.027(10)	0.034(10)	0.001(8)	-0.015(8)	0.000(8)
O2B	0.059(13)	0.081(16)	0.058(13)	0.025(12)	0.009(11)	0.030(12)
O4B	0.041(10)	0.056(12)	0.041(10)	-0.016(9)	-0.014(8)	0.006(8)
C6B	0.025(10)	0.034(12)	0.040(12)	0.004(10)	0.011(9)	0.004(9)
C8B	0.049(14)	0.022(11)	0.033(12)	-0.001(9)	0.004(10)	-0.006(10)
C3B	0.023(9)	0.034(11)	0.025(10)	0.017(8)	-0.006(8)	-0.004(9)
O5A	0.047(11)	0.067(14)	0.059(12)	0.022(11)	0.012(9)	0.022(10)
C7A	0.063(16)	0.017(10)	0.025(11)	0.008(8)	-0.004(10)	0.000(10)
O5B	0.12(2)	0.061(15)	0.050(13)	0.014(11)	0.007(13)	-0.016(14)
C4C	0.042(13)	0.019(10)	0.047(14)	0.020(10)	0.004(11)	-0.009(10)
C3C	0.044(13)	0.022(11)	0.046(14)	-0.011(10)	0.012(11)	0.018(10)
C4A	0.020(11)	0.09(2)	0.040(14)	0.015(14)	-0.022(10)	-0.003(12)

C8A	0.061(16)	0.028(12)	0.025(11)	0.007(9)	-0.017(11)	-0.011(11)
O3A	0.068(14)	0.10(2)	0.029(10)	0.002(11)	-0.005(9)	0.009(13)
C1C	0.036(13)	0.058(18)	0.033(13)	0.013(12)	0.004(10)	-0.012(12)
C2A	0.044(14)	0.055(16)	0.035(13)	-0.014(12)	-0.028(11)	0.022(13)
C5C	0.048(14)	0.058(16)	0.021(11)	0.025(11)	-0.003(10)	-0.022(13)
O2C	0.064(14)	0.075(16)	0.061(14)	0.004(12)	-0.012(11)	0.026(12)
C1B	0.020(9)	0.069(17)	0.017(10)	0.017(11)	0.002(8)	-0.008(10)
C5A	0.045(13)	0.018(10)	0.038(13)	-0.005(9)	-0.005(10)	0.006(10)
C2C	0.066(17)	0.023(11)	0.039(14)	0.012(10)	0.017(12)	-0.009(12)
N1A	0.09(2)	0.049(15)	0.046(14)	-0.017(12)	-0.033(14)	0.009(14)
C7C	0.030(12)	0.060(18)	0.042(14)	0.004(13)	0.009(10)	0.001(12)
C6C	0.034(13)	0.044(15)	0.056(16)	0.007(12)	0.013(11)	-0.004(11)
C9A	0.056(18)	0.08(2)	0.034(14)	-0.022(15)	0.009(12)	0.000(16)
C8C	0.043(6)	0.043(6)	0.043(6)	-0.0002(14)	0.0000(14)	0.0000(14)
C6A	0.040(13)	0.057(17)	0.034(13)	-0.023(12)	-0.009(10)	-0.005(12)
N1C	0.052(14)	0.075(19)	0.052(15)	0.006(14)	0.016(12)	-0.006(13)
C3A	0.057(17)	0.041(16)	0.045(15)	0.021(12)	-0.006(13)	-0.008(13)
C9C	0.047(17)	0.13(3)	0.056(19)	0.06(2)	0.017(15)	0.02(2)
C9B	0.08(2)	0.041(15)	0.018(11)	0.004(10)	0.003(12)	-0.020(14)
C7B	0.039(13)	0.046(14)	0.041(13)	-0.006(11)	0.004(11)	-0.015(12)
C5B	0.044(14)	0.052(16)	0.032(12)	-0.008(11)	-0.002(11)	-0.014(12)

Table S5. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for Cyt_PW_20240717 compound **2**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)

Supplementary Information

W1	0.57710(10)	0.28997(10)	0.78065(15)	0.0308(6)
W2	0.38017(10)	0.61625(10)	0.16036(15)	0.0301(6)
W3	0.61979(10)	0.38376(10)	0.16032(15)	0.0297(6)
W4	0.42284(10)	0.71000(10)	0.78051(15)	0.0317(6)
W5	0.52492(11)	0.19473(11)	0.97843(16)	0.0354(6)
W6	0.53193(11)	0.34348(11)	0.97580(16)	0.0361(6)
W7	0.46805(11)	0.65660(12)	0.97600(16)	0.0364(7)
W8	0.61098(11)	0.07879(11)	0.35675(16)	0.0378(7)
W9	0.60919(12)	0.08510(11)	0.68498(17)	0.0385(7)
W10	0.47501(11)	0.80517(11)	0.97859(16)	0.0366(7)
W11	0.46523(12)	0.07734(11)	0.35713(17)	0.0392(7)
W12	0.38919(11)	0.92120(11)	0.35675(17)	0.0382(7)
W13	0.42043(12)	0.83761(11)	0.52752(17)	0.0384(7)
W14	0.39092(12)	0.91493(11)	0.68504(17)	0.0389(7)
W15	0.53482(12)	0.92262(11)	0.35717(17)	0.0394(7)
W16	0.47349(12)	0.08357(11)	0.68508(17)	0.0397(7)
W17	0.52659(12)	0.91642(11)	0.68497(17)	0.0400(7)
W18	0.64113(11)	0.00199(11)	0.51481(18)	0.0397(7)
W19	0.57956(12)	0.16227(11)	0.52752(17)	0.0382(7)
W20	0.35895(11)	0.99812(11)	0.51489(18)	0.0400(7)
P2	0.666667	0.333333	0.9761(13)	0.004000
P3	0.333333	0.666667	0.9767(13)	0.004000
P1	0.4998(6)	0.9996(6)	0.5194(8)	0.004000
O4	0.5812(15)	0.0018(15)	0.304(2)	0.032(9)
O5	0.4184(17)	0.9984(15)	0.306(2)	0.040(10)
O13A	0.6313(14)	0.2683(14)	0.005(2)	0.025(8)
O2B	0.3682(15)	0.7316(15)	0.006(2)	0.031(8)

O6	0.6043(16)	0.9405(17)	0.427(2)	0.038(9)
O7	0.4511(14)	0.9993(14)	0.467(2)	0.027(8)
O3B	0.4866(14)	0.7394(14)	0.005(2)	0.023(8)
O1A	0.5512(15)	0.3277(15)	0.860(2)	0.030(8)
O8	0.3715(16)	0.8442(14)	0.615(2)	0.036(10)
O9	0.3973(16)	0.0605(16)	0.428(2)	0.041(10)
O2A	0.5144(16)	0.2616(18)	0.003(2)	0.037(10)
O4B	0.3952(14)	0.5997(14)	0.261(2)	0.026(8)
O5B	0.4489(14)	0.6714(14)	0.861(2)	0.026(8)
O10	0.6593(15)	0.1266(18)	0.279(3)	0.046(11)
O6B	0.4530(17)	0.7727(15)	0.863(2)	0.034(9)
O11	0.3350(17)	0.9370(15)	0.425(2)	0.038(10)
O12	0.5231(16)	0.1550(15)	0.617(3)	0.042(10)
O13	0.5275(16)	0.0575(17)	0.580(2)	0.043(10)
O3A	0.6028(15)	0.3984(15)	0.258(2)	0.034(9)
O4A	0.5198(18)	0.2623(18)	0.709(3)	0.050(12)
O14	0.4757(17)	0.8466(16)	0.617(2)	0.040(9)
O15	0.5878(16)	0.9427(15)	0.596(2)	0.039(10)
O5A	0.5466(16)	0.2257(15)	0.862(2)	0.035(9)
O16	0.5365(15)	0.0714(16)	0.331(2)	0.035(9)
O6A	0.6308(16)	0.2646(16)	0.741(2)	0.039(9)
O17	0.3846(15)	0.8670(15)	0.449(2)	0.033(9)
O18	0.3850(16)	0.7644(14)	0.505(2)	0.033(10)
O19	0.4631(15)	0.9287(16)	0.331(2)	0.035(9)
O20	0.6450(16)	0.0609(16)	0.595(2)	0.033(9)
O7B	0.4528(17)	0.6404(17)	0.097(2)	0.041(10)
O7A	0.4546(19)	0.1369(19)	0.970(3)	0.053(12)

O21	0.7066(18)	0.0032(18)	0.537(2)	0.046(11)
O22	0.6289(17)	0.1558(16)	0.616(2)	0.044(11)
O23	0.6658(17)	0.0638(17)	0.428(2)	0.042(10)
O24	0.3433(18)	0.8741(15)	0.279(3)	0.047(11)
O25	0.5493(16)	0.0015(15)	0.464(2)	0.039(10)
O26	0.4871(17)	0.8692(15)	0.450(3)	0.045(11)
O8B	0.3649(15)	0.6307(15)	0.740(2)	0.033(9)
O27	0.3551(16)	0.9391(16)	0.595(2)	0.034(9)
O28	0.6147(16)	0.1340(16)	0.447(2)	0.037(10)
O48	0.5123(16)	0.1316(15)	0.447(3)	0.044(10)
O8A	0.5825(18)	0.4284(18)	0.960(2)	0.045(11)
O29	0.5468(16)	0.0951(17)	0.739(2)	0.041(9)
O9A	0.7016(17)	0.3985(19)	0.174(2)	0.051(11)
O10A	0.5462(17)	0.3598(17)	0.095(2)	0.041(10)
O9B	0.4302(17)	0.8456(16)	0.963(2)	0.050(11)
O30	0.2945(19)	0.9970(18)	0.537(3)	0.052(12)
O31	0.667(2)	0.1149(19)	0.761(3)	0.056(12)
O32	0.4129(17)	0.0589(17)	0.597(2)	0.043(10)
O33	0.4550(16)	0.9046(16)	0.738(2)	0.039(9)
O34	0.4752(17)	0.9448(17)	0.580(3)	0.048(10)
O35	0.6155(17)	0.2363(16)	0.503(3)	0.039(10)
O11A	0.5390(16)	0.1924(14)	0.095(2)	0.030(9)
O36	0.5375(18)	0.8769(17)	0.278(3)	0.057(13)
O12A	0.666667	0.333333	0.872(3)	0.0130(19)
O37	0.5656(17)	0.9985(16)	0.714(3)	0.053(13)
O10B	0.5363(18)	0.6635(19)	0.966(3)	0.054(11)
O11B	0.4618(16)	0.8091(16)	0.097(2)	0.038(9)

O38	0.5536(19)	0.8900(19)	0.759(3)	0.058(12)
O12B	0.4002(18)	0.6987(17)	0.173(2)	0.042(10)
O39	0.4352(19)	0.0011(17)	0.715(3)	0.061(13)
O40	0.446(2)	0.110(2)	0.763(3)	0.060(12)
O13B	0.333333	0.666667	0.875(4)	0.024(14)
O21B	0.4821(19)	0.7370(19)	0.713(3)	0.054(11)
O22B	0.5445(19)	0.8610(18)	0.971(3)	0.058(12)
O21A	0.462(2)	0.334(2)	0.965(3)	0.064(13)
O1	0.4638(18)	0.1251(17)	0.280(3)	0.059(13)
C209	0.492(3)	0.247(2)	0.509(3)	0.034(13)
C109	0.510(2)	0.752(2)	0.506(3)	0.029(13)
O301	0.3340(18)	0.8861(17)	0.761(3)	0.052(12)
N101	0.616(3)	0.792(3)	0.513(5)	0.089(18)
N203	0.386(4)	0.210(4)	0.516(5)	0.099(19)
O205	0.348(2)	0.215(3)	0.655(4)	0.091(17)
O105	0.649(3)	0.786(2)	0.655(4)	0.095(18)
C108	0.566(3)	0.777(3)	0.543(4)	0.044(14)
O204	0.324(3)	0.181(2)	0.392(4)	0.091(16)
N102	0.475(2)	0.738(2)	0.354(3)	0.053(14)
N202	0.532(2)	0.265(2)	0.353(3)	0.054(14)
O104	0.678(3)	0.821(3)	0.391(5)	0.12(3)
C107	0.669(3)	0.810(3)	0.565(5)	0.059(16)
O103	0.776(2)	0.899(3)	0.579(5)	0.13(2)
C208	0.437(3)	0.226(3)	0.544(4)	0.049(15)
N103	0.571(3)	0.779(3)	0.375(4)	0.090(18)
C106	0.623(4)	0.800(4)	0.426(6)	0.077(19)
O102	0.622(3)	0.774(3)	0.847(5)	0.13(2)

N201	0.420(2)	0.216(3)	0.381(5)	0.104(19)
C105	0.517(3)	0.757(3)	0.406(3)	0.066(17)
C207	0.486(2)	0.246(3)	0.409(3)	0.066(17)
O203	0.223(2)	0.102(3)	0.579(5)	0.14(3)
C206	0.374(2)	0.199(3)	0.436(6)	0.074(18)
O201	0.378(3)	0.224(3)	0.846(5)	0.14(2)
C205	0.336(4)	0.193(3)	0.568(6)	0.078(19)
C104	0.693(4)	0.891(4)	0.658(6)	0.10(2)
C204	0.328(4)	0.165(4)	0.718(6)	0.09(2)
O202	0.264(3)	0.053(3)	0.716(4)	0.12(2)
C103	0.630(4)	0.821(4)	0.790(6)	0.10(2)
C203	0.369(3)	0.182(3)	0.789(5)	0.072(18)
C102	0.674(4)	0.833(4)	0.720(5)	0.08(2)
C101	0.719(4)	0.886(4)	0.576(6)	0.10(2)
C202	0.286(4)	0.112(4)	0.589(6)	0.09(2)
O101	0.736(3)	0.945(4)	0.716(5)	0.15(2)
C201	0.313(4)	0.111(4)	0.666(6)	0.11(2)
O1X	0.445(3)	0.222(3)	0.194(5)	0.14(2)
O2X	0.552(3)	0.775(3)	0.187(4)	0.12(2)
O3X	0.333333	0.666667	0.370(7)	0.102(4)

Table S6. Bond lengths (Å) for compound **2**.

W1-O4A	1.67(4)	W1-O1A	1.85(3)
W1-O6A	1.87(3)	W1-O5A	1.88(3)
W1-O6A#4	1.89(3)	W1-O12A	2.41(3)
W2-O4B	1.69(3)	W2-O7B	1.89(4)
W2-O12B	1.89(4)	W2-O12B#3	1.90(3)

W2-O11B#3	1.97(4)	W2-O2B#3	2.46(3)
W3-O3A	1.65(3)	W3-O9A#1	1.87(4)
W3-O9A	1.92(4)	W3-O10A	1.93(4)
W3-O11A#4	1.97(4)	W3-O13A#4	2.48(3)
W4-O21B	1.66(4)	W4-O8B#2	1.85(3)
W4-O6B	1.87(3)	W4-O5B	1.88(3)
W4-O8B	1.90(3)	W4-O13B	2.43(4)
W5-O7A	1.65(4)	W5-O11A	1.82(4)
W5-O2A	1.88(4)	W5-O5A	1.91(3)
W5-O8A#1	1.94(4)	W5-O13A	2.42(3)
W6-O21A	1.66(4)	W6-O10A	1.86(4)
W6-O8A	1.89(4)	W6-O1A	1.94(3)
W6-O2A	1.93(4)	W6-O13A#4	2.45(3)
W7-O10B	1.65(4)	W7-O7B	1.89(4)
W7-O5B	1.91(3)	W7-O9B#3	1.93(4)
W7-O3B	1.96(3)	W7-O2B#3	2.44(3)
W8-O10	1.70(4)	W8-O16	1.84(3)
W8-O4	1.89(3)	W8-O28	1.93(3)
W8-O23	1.94(4)	W8-O25	2.43(3)
W9-O31	1.71(4)	W9-O20	1.91(3)
W9-O29	1.91(4)	W9-O22	1.92(4)
W9-O37	1.95(4)	W9-O13	2.43(4)
W10-O22B	1.62(4)	W10-O11B	1.85(4)
W10-O3B	1.87(3)	W10-O9B	1.88(4)
W10-O6B	1.91(3)	W10-O2B	2.43(3)
W11-O1	1.70(4)	W11-O48	1.89(4)
W11-O9	1.89(4)	W11-O5	1.91(3)

W11-O16	1.93(3)	W11-O7	2.47(3)
W12-O24	1.68(4)	W12-O19	1.83(3)
W12-O5	1.87(3)	W12-O11	1.91(4)
W12-O17	1.93(3)	W12-O7	2.47(3)
W13-O18	1.64(3)	W13-O17	1.87(3)
W13-O26	1.88(4)	W13-O14	1.89(4)
W13-O8	1.89(4)	W13-O34	2.48(4)
W14-O301	1.70(4)	W14-O27	1.91(3)
W14-O8	1.93(3)	W14-O39	1.94(4)
W14-O33	1.94(4)	W14-O34	2.47(4)
W15-O36	1.70(4)	W15-O6	1.90(4)
W15-O26	1.92(4)	W15-O4	1.93(3)
W15-O19	1.94(3)	W15-O25	2.46(3)
W16-O40	1.67(4)	W16-O39	1.86(4)
W16-O32	1.89(4)	W16-O12	1.91(4)
W16-O29	1.92(4)	W16-O13	2.41(4)
W17-O38	1.63(4)	W17-O37	1.85(3)
W17-O33	1.87(4)	W17-O14	1.90(4)
W17-O15	1.91(4)	W17-O34	2.39(4)
W18-O21	1.68(4)	W18-O15	1.89(3)
W18-O20	1.89(3)	W18-O6	1.91(4)
W18-O23	1.91(3)	W18-O25	2.45(4)
W19-O35	1.67(3)	W19-O28	1.86(3)
W19-O22	1.90(4)	W19-O48	1.92(4)
W19-O12	1.92(4)	W19-O13	2.43(4)
W20-O30	1.65(4)	W20-O27	1.89(3)
W20-O9	1.92(4)	W20-O32	1.93(3)

W20-O11	1.93(3)	W20-O7	2.43(3)
P2-O13A	1.49(3)	P2-O13A#1	1.49(3)
P2-O13A#4	1.49(3)	P2-O12A	1.59(5)
P3-O2B#2	1.49(3)	P3-O2B#3	1.49(3)
P3-O2B	1.49(3)	P3-O13B	1.56(6)
P1-O7	1.47(3)	P1-O25	1.50(4)
P1-O34	1.52(4)	P1-O13	1.57(4)
C209-C208	1.32(8)	C209-C207	1.543(15)
C109-C108	1.36(7)	C109-C105	1.543(15)
N101-C108	1.22(8)	N101-C106	1.34(9)
N101-C107	1.43(9)	N203-C208	1.21(9)
N203-C206	1.27(9)	N203-C205	1.37(10)
O205-C205	1.42(9)	O205-C204	1.47(9)
O105-C102	1.44(9)	O105-C107	1.48(8)
O204-C206	1.30(7)	N102-C105	1.21(7)
N202-C207	1.31(6)	O104-C106	1.33(9)
C107-C101	1.71(10)	O103-C101	1.33(9)
N103-C105	1.28(8)	N103-C106	1.41(9)
O102-C103	1.41(9)	N201-C206	1.31(7)
N201-C207	1.53(7)	O203-C202	1.47(9)
O201-C203	1.30(9)	C205-C202	1.82(10)
C104-C101	1.45(11)	C104-O101	1.53(10)
C104-C102	1.59(11)	C204-C201	1.45(12)
C204-C203	1.43(10)	O202-C201	1.57(10)
C103-C102	1.46(11)	C202-C201	1.37(11)

Table S7. Bond angles (°) for compound **2**.

Supplementary Information

O4A-W1-O1A	100.8(18)	O4A-W1-O6A	105.7(18)
O1A-W1-O6A	153.5(15)	O4A-W1-O5A	100.1(18)
O1A-W1-O5A	85.2(15)	O6A-W1-O5A	88.5(15)
O4A-W1-O6A#4	105.8(18)	O1A-W1-O6A#4	86.6(15)
O6A-W1-O6A#4	88.(2)	O5A-W1-O6A#4	153.8(15)
O4A-W1-O12A	174.4(18)	O1A-W1-O12A	83.2(12)
O6A-W1-O12A	70.5(13)	O5A-W1-O12A	84.1(13)
O6A#4-W1-O12A	70.3(13)	O4B-W2-O7B	104.2(16)
O4B-W2-O12B	102.1(15)	O7B-W2-O12B	90.9(16)
O4B-W2-O12B#3	101.9(14)	O7B-W2-O12B#3	153.9(15)
O12B-W2-O12B#3	84.(2)	O4B-W2-O11B#3	103.6(15)
O7B-W2-O11B#3	85.8(15)	O12B-W2-O11B#3	154.2(14)
O12B#3-W2-O11B#3	87.9(16)	O4B-W2-O2B#3	172.5(13)
O7B-W2-O2B#3	71.0(14)	O12B-W2-O2B#3	84.0(13)
O12B#3-W2-O2B#3	83.0(13)	O11B#3-W2-O2B#3	70.7(13)
O3A-W3-O9A#1	101.0(16)	O3A-W3-O9A	103.3(16)
O9A#1-W3-O9A	82.(3)	O3A-W3-O10A	103.0(15)
O9A#1-W3-O10A	92.5(17)	O9A-W3-O10A	153.7(14)
O3A-W3-O11A#4	105.7(15)	O9A#1-W3-O11A#4	153.0(14)
O9A-W3-O11A#4	88.6(16)	O10A-W3-O11A#4	85.3(14)
O3A-W3-O13A#4	171.8(14)	O9A#1-W3-O13A#4	84.8(14)
O9A-W3-O13A#4	83.2(13)	O10A-W3-O13A#4	70.7(12)
O11A#4-W3-O13A#4	69.1(12)	O21B-W4-O8B#2	108.5(18)
O21B-W4-O6B	99.9(18)	O8B#2-W4-O6B	90.0(15)
O21B-W4-O5B	98.2(17)	O8B#2-W4-O5B	153.3(14)
O6B-W4-O5B	84.1(14)	O21B-W4-O8B	107.1(18)
O8B#2-W4-O8B	86.(2)	O6B-W4-O8B	152.5(15)

Supplementary Information

O5B-W4-O8B	87.1(14)	O21B-W4-O13B	177.3(18)
O8B#2-W4-O13B	71.0(13)	O6B-W4-O13B	82.8(14)
O5B-W4-O13B	82.4(13)	O8B-W4-O13B	70.3(13)
O7A-W5-O11A	100.9(17)	O7A-W5-O2A	103.7(18)
O11A-W5-O2A	87.4(14)	O7A-W5-O5A	104.6(17)
O11A-W5-O5A	154.5(15)	O2A-W5-O5A	87.4(15)
O7A-W5-O8A#1	101.1(17)	O11A-W5-O8A#1	86.8(15)
O2A-W5-O8A#1	155.1(15)	O5A-W5-O8A#1	87.5(15)
O7A-W5-O13A	170.6(15)	O11A-W5-O13A	72.6(13)
O2A-W5-O13A	83.0(13)	O5A-W5-O13A	82.0(13)
O8A#1-W5-O13A	72.2(13)	O21A-W6-O10A	101.6(19)
O21A-W6-O8A	102.8(19)	O10A-W6-O8A	85.8(16)
O21A-W6-O1A	103.7(18)	O10A-W6-O1A	154.5(14)
O8A-W6-O1A	91.2(15)	O21A-W6-O2A	101.7(19)
O10A-W6-O2A	86.9(15)	O8A-W6-O2A	155.4(15)
O1A-W6-O2A	85.4(14)	O21A-W6-O13A#4	172.4(17)
O10A-W6-O13A#4	72.5(13)	O8A-W6-O13A#4	72.3(13)
O1A-W6-O13A#4	82.4(12)	O2A-W6-O13A#4	83.0(13)
O10B-W7-O7B	101.5(18)	O10B-W7-O5B	104.5(17)
O7B-W7-O5B	154.0(14)	O10B-W7-O9B#3	101.7(18)
O7B-W7-O9B#3	84.6(16)	O5B-W7-O9B#3	91.6(15)
O10B-W7-O3B	103.2(17)	O7B-W7-O3B	85.5(15)
O5B-W7-O3B	8 7.2(13)	O9B#3-W7-O3B	154.6(15)
O10B-W7-O2B#3	170.3(17)	O7B-W7-O2B#3	71.4(14)
O5B-W7-O2B#3	83.0(12)	O9B#3-W7-O2B#3	71.6(14)
O3B-W7-O2B#3	83.1(12)	O10-W8-O16	105.0(17)
O10-W8-O4	102.0(17)	O16-W8-O4	86.7(15)

O10-W8-O28	103.2(17)	O16-W8-O28	84.5(15)
O4-W8-O28	154.7(15)	O10-W8-O23	101.5(16)
O16-W8-O23	153.4(15)	O4-W8-O23	89.6(15)
O28-W8-O23	87.7(15)	O10-W8-O25	171.4(15)
O16-W8-O25	81.3(14)	O4-W8-O25	72.2(13)
O28-W8-O25	83.1(14)	O23-W8-O25	72.5(14)
O31-W9-O20	101.4(17)	O31-W9-O29	102.9(18)
O20-W9-O29	155.7(15)	O31-W9-O22	101.3(18)
O20-W9-O22	87.4(16)	O29-W9-O22	87.8(16)
O31-W9-O37	103.(2)	O20-W9-O37	84.1(15)
O29-W9-O37	90.6(15)	O22-W9-O37	155.8(17)
O31-W9-O13	171.1(16)	O20-W9-O13	84.3(13)
O29-W9-O13	71.7(14)	O22-W9-O13	71.9(13)
O37-W9-O13	84.7(16)	O22B-W10-O11B	100.0(19)
O22B-W10-O3B	101.9(18)	O11B-W10-O3B	86.9(15)
O22B-W10-O9B	101.7(18)	O11B-W10-O9B	85.7(16)
O3B-W10-O9B	156.1(14)	O22B-W10-O6B	105.2(19)
O11B-W10-O6B	154.9(15)	O3B-W10-O6B	87.8(14)
O9B-W10-O6B	89.4(16)	O22B-W10-O2B	171.0(16)
O11B-W10-O2B	73.1(14)	O3B-W10-O2B	83.6(13)
O9B-W10-O2B	72.4(13)	O6B-W10-O2B	81.9(14)
O1-W11-O48	102.7(18)	O1-W11-O9	102.5(18)
O48-W11-O9	85.4(15)	O1-W11-O5	103.7(19)
O48-W11-O5	153.6(16)	O9-W11-O5	88.8(15)
O1-W11-O16	105.4(18)	O48-W11-O16	86.1(15)
O9-W11-O16	152.0(14)	O5-W11-O16	87.0(15)
O1-W11-O7	171.7(15)	O48-W11-O7	82.8(13)

O9-W11-O7	71.4(13)	O5-W11-O7	71.0(14)
O16-W11-O7	81.1(13)	O24-W12-O19	103.3(18)
O24-W12-O5	102.6(17)	O19-W12-O5	87.3(16)
O24-W12-O11	102.7(18)	O19-W12-O11	154.0(15)
O5-W12-O11	87.6(14)	O24-W12-O17	104.0(16)
O19-W12-O17	85.7(15)	O5-W12-O17	153.4(15)
O11-W12-O17	87.5(14)	O24-W12-O7	172.3(14)
O19-W12-O7	81.8(13)	O5-W12-O7	71.6(14)
O11-W12-O7	72.4(13)	O17-W12-O7	82.0(12)
O18-W13-O17	102.5(16)	O18-W13-O26	102.5(16)
O17-W13-O26	86.3(16)	O18-W13-O14	103.9(17)
O17-W13-O14	153.6(15)	O26-W13-O14	87.2(17)
O18-W13-O8	103.6(16)	O17-W13-O8	87.3(16)
O26-W13-O8	153.9(14)	O14-W13-O8	87.3(16)
O18-W13-O34	172.8(16)	O17-W13-O34	83.8(13)
O26-W13-O34	81.3(14)	O14-W13-O34	70.0(14)
O8-W13-O34	72.9(13)	O301-W14-O27	101.3(18)
O301-W14-O8	102.3(17)	O27-W14-O8	87.3(15)
O301-W14-O39	102.(2)	O27-W14-O39	84.9(16)
O8-W14-O39	155.4(17)	O301-W14-O33	104.1(18)
O27-W14-O33	154.6(15)	O8-W14-O33	87.0(16)
O39-W14-O33	90.1(16)	O301-W14-O34	172.2(16)
O27-W14-O34	84.6(14)	O8-W14-O34	72.7(13)
O39-W14-O34	83.3(17)	O33-W14-O34	70.1(14)
O36-W15-O6	102.3(18)	O36-W15-O26	105.8(17)
O6-W15-O26	86.2(16)	O36-W15-O4	101.3(17)
O6-W15-O4	88.8(15)	O26-W15-O4	152.8(14)

O36-W15-O19	105.4(18)	O6-W15-O19	152.3(15)
O26-W15-O19	85.7(15)	O4-W15-O19	86.4(15)
O36-W15-O25	170.0(15)	O6-W15-O25	72.0(14)
O26-W15-O25	82.3(13)	O4-W15-O25	70.8(13)
O19-W15-O25	80.7(13)	O40-W16-O39	101.(2)
O40-W16-O32	102.1(18)	O39-W16-O32	85.5(17)
O40-W16-O12	102.6(18)	O39-W16-O12	156.6(18)
O32-W16-O12	88.1(16)	O40-W16-O29	101.0(19)
O39-W16-O29	89.2(16)	O32-W16-O29	156.8(15)
O12-W16-O29	87.9(16)	O40-W16-O13	171.4(18)
O39-W16-O13	84.6(17)	O32-W16-O13	84.9(14)
O12-W16-O13	72.5(13)	O29-W16-O13	72.1(14)
O38-W17-O37	101.(2)	O38-W17-O33	101.9(19)
O37-W17-O33	90.4(15)	O38-W17-O14	103.2(19)
O37-W17-O14	155.5(18)	O33-W17-O14	86.3(16)
O38-W17-O15	101.8(18)	O37-W17-O15	84.1(16)
O33-W17-O15	156.3(15)	O14-W17-O15	89.3(16)
O38-W17-O34	173.1(18)	O37-W17-O34	83.7(17)
O33-W17-O34	73.0(15)	O14-W17-O34	72.1(14)
O15-W17-O34	83.4(14)	O21-W18-O15	101.0(17)
O21-W18-O20	101.3(17)	O15-W18-O20	86.4(16)
O21-W18-O6	103.4(17)	O15-W18-O6	87.4(16)
O20-W18-O6	155.3(15)	O21-W18-O23	102.1(18)
O15-W18-O23	156.8(16)	O20-W18-O23	86.5(15)
O6-W18-O23	90.0(16)	O21-W18-O25	172.8(15)
O15-W18-O25	84.7(14)	O20-W18-O25	83.4(13)
O6-W18-O25	72.2(13)	O23-W18-O25	72.6(14)

O35-W19-O28	100.7(17)	O35-W19-O22	104.2(17)
O28-W19-O22	88.6(16)	O35-W19-O48	100.6(16)
O28-W19-O48	85.3(16)	O22-W19-O48	155.1(14)
O35-W19-O12	103.4(16)	O28-W19-O12	155.7(15)
O22-W19-O12	88.5(17)	O48-W19-O12	87.2(15)
O35-W19-O13	173.9(16)	O28-W19-O13	84.3(14)
O22-W19-O13	72.2(14)	O48-W19-O13	83.2(13)
O12-W19-O13	71.9(13)	O30-W20-O27	101.2(17)
O30-W20-O9	104.3(17)	O27-W20-O9	154.4(15)
O30-W20-O32	100.2(17)	O27-W20-O32	86.8(16)
O9-W20-O32	86.3(16)	O30-W20-O11	102.8(17)
O27-W20-O11	87.5(14)	O9-W20-O11	89.3(15)
O32-W20-O11	156.9(16)	O30-W20-O7	174.2(15)
O27-W20-O7	82.9(13)	O9-W20-O7	72.0(13)
O32-W20-O7	84.1(13)	O11-W20-O7	73.0(13)
O13A-P2-O13A#1	111.6(13)	O13A-P2-O13A#4	111.6(13)
O13A#1-P2-O13A#4	111.6(13)	O13A-P2-O12A	107.2(14)
O13A#1-P2-O12A	107.2(14)	O13A#4-P2-O12A	107.2(14)
O2B#2-P3-O2B#3	111.2(14)	O2B#2-P3-O2B	111.2(14)
O2B#3-P3-O2B	111.2(14)	O2B#2-P3-O13B	107.7(15)
O2B#3-P3-O13B	107.7(15)	O2B-P3-O13B	107.7(15)
O7-P1-O25	112.(2)	O7-P1-O34	112.(2)
O25-P1-O34	110.(2)	O7-P1-O13	107.9(19)
O25-P1-O13	109.(2)	O34-P1-O13	106.(2)
W8-O4-W15	127.8(18)	W12-O5-W11	130.(2)
P2-O13A-W5	128.3(18)	P2-O13A-W6#1	126.6(18)
W5-O13A-W6#1	89.0(10)	P2-O13A-W3#1	123.7(19)

W5-O13A-W3#1	88.8(10)	W6#1-O13A-W3#1	87.9(10)
P3-O2B-W10	127.5(19)	P3-O2B-W7#2	126.6(19)
W10-O2B-W7#2	88.8(11)	P3-O2B-W2#2	124.(2)
W10-O2B-W2#2	88.9(11)	W7#2-O2B-W2#2	88.4(11)
W15-O6-W18	127.2(19)	P1-O7-W20	129.0(19)
P1-O7-W12	124.9(18)	W20-O7-W12	88.7(10)
P1-O7-W11	125.6(18)	W20-O7-W11	88.3(10)
W12-O7-W11	87.6(10)	W10-O3B-W7	147.2(18)
W1-O1A-W6	153.6(19)	W13-O8-W14	127.1(17)
W11-O9-W20	127.7(19)	W5-O2A-W6	149.8(19)
W4-O5B-W7	153.1(18)	W4-O6B-W10	154.1(19)
W12-O11-W20	126.(2)	W16-O12-W19	125.8(18)
P1-O13-W16	127.(2)	P1-O13-W19	125.(2)
W16-O13-W19	89.6(12)	P1-O13-W9	125.(2)
W16-O13-W9	89.7(12)	W19-O13-W9	89.2(12)
W13-O14-W17	129.(2)	W18-O15-W17	151.(2)
W1-O5A-W5	152.(2)	W8-O16-W11	154.(2)
W1-O6A-W1#1	129.(2)	W13-O17-W12	152.(2)
W12-O19-W15	154.(2)	W18-O20-W9	151.(2)
W2-O7B-W7	129.(2)	W19-O22-W9	126.7(18)
W18-O23-W8	125.3(19)	P1-O25-W8	127.(2)
P1-O25-W18	126.(2)	W8-O25-W18	89.2(12)
P1-O25-W15	124.7(19)	W8-O25-W15	89.0(12)
W18-O25-W15	88.4(12)	W13-O26-W15	152.(2)
W4#3-O8B-W4	130.0(19)	W20-O27-W14	151.(2)
W19-O28-W8	153.(2)	W11-O48-W19	151.(2)
W6-O8A-W5#4	126.4(18)	W9-O29-W16	126.(2)

W3#4-O9A-W3	154.(2)	W6-O10A-W3	128.9(18)
W10-O9B-W7#2	127.1(19)	W16-O32-W20	149.(2)
W17-O33-W14	127.(2)	P1-O34-W17	130.(2)
P1-O34-W14	125.(2)	W17-O34-W14	89.3(13)
P1-O34-W13	123.(2)	W17-O34-W13	88.8(12)
W14-O34-W13	87.2(12)	W5-O11A-W3#1	129.3(17)
P2-O12A-W1#4	125.4(9)	P2-O12A-W1	125.4(9)
W1#4-O12A-W1	89.8(13)	P2-O12A-W1#1	125.4(9)
W1#4-O12A-W1#1	89.8(13)	W1-O12A-W1#1	89.8(13)
W17-O37-W9	1 53.(3)	W10-O11B-W2#2	127.2(19)
W2-O12B-W2#2	153.(2)	W16-O39-W14	152.(3)
P3-O13B-W4#3	126.3(11)	P3-O13B-W4	126.3(11)
W4#3-O13B-W4	88.6(16)	P3-O13B-W4#2	126.3(11)
W4#3-O13B-W4#2	88.6(16)	W4-O13B-W4#2	88.6(16)
C208-C209-C207	109.(5)	C108-C109-C105	109.(5)
C108-N101-C106	118.(7)	C108-N101-C107	123.(7)
C106-N101-C107	118.(7)	C208-N203-C206	121.(8)
C208-N203-C205	124.(8)	C206-N203-C205	114.(8)
C205-O205-C204	111.(6)	C102-O105-C107	113.(6)
N101-C108-C109	132.(7)	N101-C107-O105	109.(6)
N101-C107-C101	117.(6)	O105-C107-C101	107.(6)
N203-C208-C209	136.(7)	C105-N103-C106	124.(7)
O104-C106-N101	120.(8)	O104-C106-N103	122.(8)
N101-C106-N103	118.(7)	C206-N201-C207	123.(6)
N102-C105-N103	117.(5)	N102-C105-C109	125.(6)
N103-C105-C109	118.(6)	N202-C207-N201	123.(5)
N202-C207-C209	126.(5)	N201-C207-C209	111.(4)

N203-C206-O204	131.(7)	N203-C206-N201	119.(7)
O204-C206-N201	109.(7)	N203-C205-O205	116.(7)
N203-C205-C202	119.(7)	O205-C205-C202	100.(6)
C101-C104-O101	115.(8)	C101-C104-C102	114.(8)
O101-C104-C102	104.(7)	O205-C204-C201	106.(7)
O205-C204-C203	111.(7)	C201-C204-C203	120.(8)
O102-C103-C102	114.(8)	O201-C203-C204	124.(7)
O105-C102-C103	112.(7)	O105-C102-C104	99.(6)
C103-C102-C104	119.(7)	O103-C101-C104	115.(9)
O103-C101-C107	112.(7)	C104-C101-C107	93.(7)
C201-C202-O203	126.(8)	C201-C202-C205	96.(7)
O203-C202-C205	105.(6)	C202-C201-C204	110.(9)
C202-C201-O202	105.(8)	C204-C201-O202	109.(8)

Table S8. Anisotropic atomic displacement parameters (Å2) for compound 2.

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W1	0.0327(13)	0.0334(14)	0.0262(14)	-0.0033(11)	-0.0051(11)	0.0164(12)
W2	0.0340(14)	0.0324(13)	0.0272(14)	0.0026(11)	-0.0003(11)	0.0191(12)
W3	0.0345(14)	0.0325(13)	0.0265(14)	-0.0035(11)	-0.0005(11)	0.0200(12)
W4	0.0330(13)	0.0363(14)	0.0266(14)	0.0031(11)	0.0054(11)	0.0178(12)
W5	0.0293(14)	0.0304(14)	0.0326(16)	-0.0004(12)	-0.0007(11)	0.0045(11)
W6	0.0308(14)	0.0495(16)	0.0359(16)	-0.0079(13)	-0.0041(12)	0.0261(13)
W7	0.0314(14)	0.0491(16)	0.0365(16)	0.0061(13)	0.0050(12)	0.0260(13)
W8	0.0377(15)	0.0299(14)	0.0403(17)	0.0041(12)	0.0052(13)	0.0127(13)
W9	0.0399(16)	0.0285(14)	0.0391(17)	-0.0037(12)	-0.0061(13)	0.0112(13)

W10	0.0300(14)	0.0310(14)	0.0361(16)	0.0006(12)	-0.0011(12)	0.0058(12)
W11	0.0422(16)	0.0284(14)	0.0458(18)	0.0051(12)	-0.0030(13)	0.0168(13)
W12	0.0382(15)	0.0300(14)	0.0411(17)	-0.0040(12)	-0.0046(13)	0.0131(13)
W13	0.0410(16)	0.0241(14)	0.0458(17)	0.0005(12)	0.0007(13)	0.0132(12)
W14	0.0410(16)	0.0296(15)	0.0392(17)	0.0036(12)	0.0044(13)	0.0125(13)
W15	0.0428(16)	0.0298(15)	0.0454(18)	-0.0041(12)	0.0036(13)	0.0181(13)
W16	0.0445(16)	0.0313(15)	0.0414(17)	-0.0080(12)	0.0006(13)	0.0177(13)
W17	0.0456(16)	0.0303(15)	0.0421(17)	0.0071(12)	-0.0031(13)	0.0174(13)
W18	0.0365(15)	0.0339(15)	0.0496(18)	0.0019(13)	0.0007(13)	0.0183(13)
W19	0.0396(15)	0.0219(13)	0.0475(17)	-0.0001(12)	-0.0011(13)	0.0113(12)
W20	0.0366(15)	0.0317(15)	0.0519(18)	-0.0014(13)	-0.0008(13)	0.0172(13)
O4	0.032(9)	0.032(9)	0.032(9)	0.0001(15)	-0.0002(15)	0.016(5)
O5	0.04(2)	0.02(2)	0.05(3)	-0.007(18)	0.02(2)	0.009(18)
O13A	0.025(8)	0.025(8)	0.025(8)	0.0001(15)	0.0000(15)	0.012(4)
O2B	0.031(9)	0.031(9)	0.031(9)	-0.0001(15)	0.0000(15)	0.015(4)
O6	0.039(9)	0.038(9)	0.038(9)	-0.0003(15)	0.0002(15)	0.019(5)
O7	0.027(8)	0.027(8)	0.027(8)	0.0001(15)	0.0001(15)	0.014(4)
O3B	0.023(8)	0.023(8)	0.023(8)	0.0000(15)	0.0002(15)	0.011(4)
O1A	0.030(8)	0.030(8)	0.030(8)	0.0000(15)	0.0001(15)	0.015(4)
O8	0.04(2)	0.011(19)	0.04(2)	0.010(17)	0.010(19)	-0.003(17)
O9	0.04(2)	0.02(2)	0.05(3)	0.004(19)	-0.03(2)	0.012(19)
O2A	0.03(2)	0.06(3)	0.01(2)	-0.003(19)	-0.001(17)	0.02(2)
O4B	0.026(8)	0.026(8)	0.025(9)	0.000(3)	0.000(3)	0.013(5)
O5B	0.026(8)	0.026(8)	0.026(8)	0.0001(15)	-0.0002(15)	0.013(4)
O10	0.01(2)	0.05(3)	0.07(3)	0.00(2)	0.016(19)	0.013(19)
O6B	0.07(3)	0.03(2)	0.02(2)	-0.007(16)	-0.009(19)	0.03(2)
O11	0.06(3)	0.02(2)	0.04(2)	0.001(18)	-0.01(2)	0.03(2)

O12	0.03(2)	0.02(2)	0.07(3)	-0.026(19)	-0.01(2)	0.004(17)
O13	0.043(10)	0.043(10)	0.042(10)	-0.0001(15)	0.0001(15)	0.021(5)
O3A	0.035(9)	0.035(9)	0.035(9)	0.000(3)	0.000(3)	0.018(5)
O4A	0.04(2)	0.04(2)	0.06(3)	-0.01(2)	-0.03(2)	0.02(2)
O14	0.040(10)	0.040(10)	0.040(10)	0.0000(15)	0.0000(15)	0.020(5)
O15	0.04(2)	0.02(2)	0.05(3)	0.023(19)	0.01(2)	0.005(18)
O5A	0.05(2)	0.03(2)	0.02(2)	0.003(17)	0.005(18)	0.013(19)
O16	0.035(9)	0.035(9)	0.035(9)	-0.0001(15)	0.0000(15)	0.017(5)
O6A	0.039(9)	0.039(9)	0.039(9)	-0.0001(15)	0.0000(15)	0.019(5)
O17	0.02(2)	0.02(2)	0.05(2)	0.001(18)	-0.010(18)	0.012(17)
O18	0.04(2)	0.014(19)	0.05(3)	0.005(17)	0.008(19)	0.016(18)
O19	0.035(9)	0.035(9)	0.035(9)	0.0001(15)	0.0001(15)	0.018(5)
O20	0.033(9)	0.033(9)	0.033(9)	-0.0001(15)	0.0001(15)	0.016(5)
O7B	0.042(10)	0.042(10)	0.041(10)	-0.0002(15)	0.0000(15)	0.021(5)
O7A	0.06(3)	0.07(3)	0.05(3)	0.03(2)	0.00(2)	0.04(2)
O21	0.046(11)	0.046(11)	0.046(11)	-0.001(3)	0.001(3)	0.023(6)
O22	0.05(2)	0.02(2)	0.05(3)	-0.016(19)	-0.02(2)	0.009(19)
O23	0.05(3)	0.05(2)	0.03(2)	0.02(2)	0.01(2)	0.02(2)
O24	0.05(3)	0.012(19)	0.07(3)	0.00(2)	-0.01(2)	0.010(19)
O25	0.04(2)	0.02(2)	0.04(3)	0.002(18)	0.002(19)	0.008(18)
O26	0.04(2)	0.02(2)	0.08(3)	-0.01(2)	0.02(2)	0.019(19)
O8B	0.033(9)	0.033(9)	0.033(9)	-0.0002(15)	0.0001(15)	0.017(5)
O27	0.034(9)	0.034(9)	0.034(9)	0.0003(15)	-0.0003(15)	0.017(5)
O28	0.05(2)	0.04(2)	0.04(2)	-0.008(19)	0.002(19)	0.03(2)
O48	0.04(2)	0.02(2)	0.07(3)	0.01(2)	0.02(2)	0.009(18)
O8A	0.07(3)	0.07(3)	0.03(2)	0.00(2)	-0.02(2)	0.05(2)
O29	0.041(9)	0.040(9)	0.040(10)	-0.0003(15)	0.0001(15)	0.020(5)

O9A	0.04(3)	0.07(3)	0.03(3)	-0.02(2)	0.01(2)	0.02(2)
O10A	0.05(2)	0.06(3)	0.04(2)	0.02(2)	0.03(2)	0.04(2)
O9B	0.05(2)	0.03(2)	0.04(3)	0.016(19)	0.00(2)	-0.004(19)
O30	0.07(3)	0.04(2)	0.05(3)	0.00(2)	-0.03(2)	0.03(2)
O31	0.07(3)	0.07(3)	0.05(3)	-0.02(2)	-0.02(2)	0.04(3)
O32	0.05(2)	0.04(2)	0.03(2)	-0.017(19)	-0.002(19)	0.01(2)
O33	0.039(9)	0.039(9)	0.039(9)	0.0000(15)	0.0001(15)	0.019(5)
O34	0.048(10)	0.048(10)	0.048(10)	0.0000(15)	-0.0001(15)	0.024(5)
O35	0.04(2)	0.04(2)	0.06(3)	0.01(2)	0.01(2)	0.03(2)
O11A	0.04(2)	0.014(18)	0.03(2)	0.007(17)	0.030(18)	0.015(17)
O36	0.04(3)	0.03(2)	0.09(3)	0.00(2)	0.03(2)	0.01(2)
O12A	0.0130(18)	0.0130(18)	0.013(2)	0.000000	0.000000	0.0065(9)
O37	0.03(2)	0.02(2)	0.09(3)	-0.01(2)	0.04(2)	0.000(18)
O10B	0.06(3)	0.07(3)	0.04(3)	0.00(2)	0.01(2)	0.04(2)
O11B	0.038(10)	0.038(10)	0.038(10)	0.0001(15)	-0.0002(15)	0.019(5)
O38	0.058(12)	0.057(12)	0.058(12)	0.001(3)	-0.001(3)	0.029(7)
O12B	0.07(3)	0.06(3)	0.02(2)	-0.020(19)	-0.02(2)	0.05(2)
O39	0.06(3)	0.03(2)	0.08(3)	0.00(2)	-0.03(3)	0.01(2)
O40	0.060(13)	0.059(13)	0.060(13)	0.000(3)	0.000(3)	0.030(7)
O13B	0.006(18)	0.006(18)	0.06(4)	0.000000	0.000000	0.003(9)
O21B	0.054(12)	0.054(12)	0.054(12)	0.000(3)	0.000(3)	0.027(6)
O22B	0.06(3)	0.05(3)	0.06(3)	0.00(2)	0.01(2)	0.03(2)
O21A	0.06(3)	0.09(3)	0.05(3)	0.00(3)	-0.01(2)	0.05(3)
O1	0.05(3)	0.03(2)	0.09(4)	0.02(2)	-0.01(2)	0.02(2)
C209	0.034(13)	0.034(13)	0.034(13)	0.0000(15)	0.0000(15)	0.017(7)
C109	0.029(13)	0.029(13)	0.029(13)	0.0000(15)	0.0000(15)	0.015(6)
O301	0.04(3)	0.04(2)	0.06(3)	0.01(2)	0.02(2)	0.01(2)

N101	0.089(18)	0.089(18)	0.089(18)	0.0000(15)	-0.0001(15)	0.045(9)
N203	0.099(19)	0.099(19)	0.099(19)	0.0000(15)	0.0000(15)	0.049(10)
O205	0.10(4)	0.10(4)	0.10(4)	0.02(4)	-0.01(3)	0.07(4)
O105	0.12(5)	0.08(4)	0.13(5)	-0.03(4)	-0.01(4)	0.09(4)
C108	0.044(14)	0.044(14)	0.044(14)	-0.0001(15)	0.0000(15)	0.022(7)
O204	0.091(17)	0.092(17)	0.091(17)	0.001(3)	-0.001(3)	0.046(9)
N102	0.053(15)	0.053(15)	0.053(15)	0.000(3)	-0.001(3)	0.027(8)
N202	0.054(14)	0.054(14)	0.054(15)	0.000(3)	0.000(3)	0.027(8)
O104	0.09(4)	0.10(4)	0.18(6)	0.00(4)	0.09(4)	0.05(4)
C107	0.059(16)	0.059(16)	0.059(16)	0.0000(15)	0.0000(15)	0.030(8)
O103	0.04(3)	0.12(5)	0.19(7)	0.03(5)	0.02(4)	0.01(3)
C208	0.049(15)	0.049(15)	0.049(15)	0.0000(15)	-0.0001(15)	0.024(8)
N103	0.090(18)	0.090(18)	0.090(18)	0.0001(15)	0.0000(15)	0.045(9)
C106	0.077(19)	0.077(19)	0.077(19)	0.0000(15)	0.0001(15)	0.038(9)
O102	0.13(2)	0.13(2)	0.13(2)	0.000(3)	0.000(3)	0.067(11)
N201	0.104(19)	0.104(19)	0.104(19)	0.0000(15)	-0.0001(15)	0.052(10)
C105	0.067(17)	0.066(17)	0.067(17)	0.0000(15)	-0.0001(15)	0.033(9)
C207	0.066(17)	0.066(17)	0.066(17)	0.0000(15)	0.0001(15)	0.033(9)
O203	0.04(3)	0.08(4)	0.25(8)	-0.01(5)	-0.02(4)	0.00(3)
C206	0.074(18)	0.074(18)	0.074(18)	0.0000(15)	-0.0001(15)	0.037(9)
O201	0.14(2)	0.14(2)	0.14(2)	0.000(3)	0.000(3)	0.071(12)
C205	0.078(19)	0.078(19)	0.078(19)	0.0000(15)	0.0000(15)	0.039(10)
C104	0.10(2)	0.10(2)	0.10(2)	0.0000(15)	0.0000(15)	0.050(11)
C204	0.09(2)	0.09(2)	0.09(2)	0.0000(15)	0.0001(15)	0.045(10)
O202	0.12(2)	0.12(2)	0.12(2)	0.000(3)	0.000(3)	0.061(10)
C103	0.10(2)	0.10(2)	0.10(2)	0.0000(15)	0.0000(15)	0.051(11)
C203	0.072(18)	0.072(18)	0.072(18)	0.0000(15)	0.0000(15)	0.036(9)

C102	0.08(2)	0.08(2)	0.08(2)	0.0000(15)	-0.0001(15)	0.041(10)
C101	0.10(2)	0.10(2)	0.10(2)	0.0000(15)	0.0000(15)	0.049(11)
C202	0.09(2)	0.09(2)	0.09(2)	-0.0001(15)	0.0000(15)	0.043(10)
O101	0.15(2)	0.15(2)	0.15(2)	0.000(3)	0.000(3)	0.075(13)
C201	0.11(2)	0.11(2)	0.11(2)	0.0000(15)	0.0000(15)	0.055(11)
O1X	0.14(2)	0.14(2)	0.14(2)	0.000(3)	0.000(3)	0.069(12)
O2X	0.12(2)	0.12(2)	0.12(2)	0.000(3)	0.000(3)	0.058(10)
O3X	0.102(4)	0.102(4)	0.101(5)	0.000000	0.000000	0.0508(18)

Table S9. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å2) for compound 2.

	x/a	y/b	z/c	U(eq)
H209	0.5277	0.2608	0.5408	0.041000
H109	0.4729	0.7356	-0.4635	0.035000
H10C	0.5664	0.7844	-0.3969	0.052000
H10D	0.6915	0.7909	-0.4591	0.071000
H208	0.4374	0.2231	0.6043	0.058000
H20D	0.1987	0.0656	0.5882	0.203000
H20E	0.3112	0.2078	0.5397	0.093000
H10G	0.6567	0.8931	-0.3539	0.121000
H20F	0.2890	0.1582	0.7422	0.108000
H10H	0.6438	0.8581	-0.1763	0.122000
H10I	0.5912	0.8105	-0.2359	0.122000
H20A	0.3577	0.1449	0.8217	0.086000
H20B	0.4091	0.1940	0.7634	0.086000
H10J	0.7109	0.8356	-0.2545	0.100000
H10K	0.7126	0.9098	-0.4700	0.117000

H20I	0.2928	0.0878	0.5452	0.103000
H20J	0.3499	0.1084	0.6551	0.131000

Table S10. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for compound 3.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)
W001	0.44002(9)	0.45575(6)	0.79314(5)	0.0349(3)
W002	0.37883(10)	0.81362(7)	0.69584(5)	0.0373(3)
W003	0.57985(10)	0.51674(6)	0.69664(7)	0.0438(3)
W004	0.54797(10)	0.70257(6)	0.64537(6)	0.0391(3)
W005	0.62046(11)	0.75814(6)	0.79004(6)	0.0448(3)
W006	0.65300(10)	0.57198(6)	0.84095(7)	0.0467(4)
W007	0.31981(12)	0.57597(8)	0.59400(5)	0.0471(4)
W008	0.18069(10)	0.51452(8)	0.69049(6)	0.0477(4)
W009	0.15052(10)	0.68737(9)	0.64460(6)	0.0481(4)
W00A	0.25640(12)	0.57595(8)	0.84565(6)	0.0484(4)
W00B	0.22893(13)	0.74897(8)	0.80057(6)	0.0558(4)
W00C	0.46918(15)	0.69114(7)	0.89442(5)	0.0564(4)
P00D	0.4026(5)	0.6343(3)	0.7442(2)	0.0195(11)
O00E	0.3122(16)	0.4680(11)	0.7308(9)	0.040(3)
O00F	0.2609(16)	0.7586(12)	0.6504(8)	0.041(3)
O00G	0.6052(16)	0.6099(11)	0.6748(11)	0.045(3)
O00H	0.313(2)	0.8017(12)	0.7602(9)	0.049(3)
O00I	0.3654(16)	0.5082(11)	0.8384(9)	0.038(3)
O00J	0.5195(16)	0.4434(10)	0.7346(10)	0.041(3)
O00K	0.5172(18)	0.8285(10)	0.7520(9)	0.045(3)

O00L	0.366(2)	0.6207(12)	0.9073(9)	0.056(3)
O00M	0.5442(18)	0.7473(10)	0.8491(9)	0.046(3)
O00N	0.4192(17)	0.6534(12)	0.6034(9)	0.042(3)
O00O	0.4600(17)	0.7860(11)	0.6404(9)	0.041(3)
O00P	0.3612(16)	0.6541(10)	0.7971(8)	0.036(2)
O00Q	0.4411(18)	0.5210(11)	0.6394(10)	0.047(3)
O00R	0.6444(17)	0.7425(11)	0.7137(11)	0.047(3)
O00S	0.1533(19)	0.7120(14)	0.7241(10)	0.054(4)
O00T	0.5646(19)	0.6186(11)	0.8842(10)	0.048(4)
O00U	0.6702(16)	0.6632(10)	0.8115(10)	0.046(4)
O00V	0.2012(18)	0.6448(13)	0.5825(9)	0.051(3)
O00W	0.4821(15)	0.5722(10)	0.7610(9)	0.034(2)
O00X	0.2270(19)	0.5085(14)	0.6192(9)	0.054(4)
O00Y	0.5750(16)	0.4879(11)	0.8469(9)	0.042(3)
O00Z	0.4595(15)	0.6984(10)	0.7271(8)	0.034(2)
O010	0.0843(18)	0.4506(15)	0.6807(11)	0.062(5)
O011	0.1830(17)	0.5501(13)	0.7669(10)	0.049(4)
O012	0.4291(18)	0.3715(11)	0.8176(10)	0.048(4)
O013	0.6824(16)	0.5330(10)	0.7724(11)	0.047(3)
O014	0.351(2)	0.7554(12)	0.8713(9)	0.059(4)
O015	0.3417(19)	0.8982(12)	0.6728(9)	0.048(4)
O016	0.0382(19)	0.7295(15)	0.6042(11)	0.062(5)
O017	0.184(2)	0.6650(14)	0.8349(10)	0.059(4)
O018	0.657(2)	0.4680(12)	0.6624(13)	0.064(6)
O01A	0.0964(17)	0.5951(14)	0.6562(10)	0.058(4)
O01C	0.729(2)	0.8079(12)	0.8270(12)	0.065(5)
O01E	0.534(3)	0.7178(14)	0.9651(10)	0.081(7)

O01F	0.309(2)	0.5473(15)	0.5240(10)	0.069(6)
O01G	0.7736(19)	0.5606(11)	0.8949(13)	0.064(6)
O01H	0.185(2)	0.5319(16)	0.8869(12)	0.073(6)
O01I	0.140(3)	0.8098(16)	0.8143(13)	0.091(7)
O19	0.3082(15)	0.6126(11)	0.6914(8)	0.035(2)
O1	0.6138(18)	0.7181(12)	0.5929(11)	0.052(5)
O1Z	0.440(3)	0.1912(17)	0.5550(16)	0.035(4)
C25	0.440(3)	0.1912(17)	0.5550(16)	0.035(4)
N1	0.763(5)	0.206(3)	0.496(3)	0.025(6)
N2	0.655(5)	0.263(3)	0.539(3)	0.026(8)
N3	0.507(4)	0.023(3)	0.426(2)	0.016(5)
N4	0.480(4)	0.112(3)	0.485(2)	0.016(5)
N5	0.631(4)	0.106(3)	0.462(2)	0.016(5)
C1	0.672(6)	0.167(3)	0.488(3)	0.021(8)
C2	0.604(6)	0.201(3)	0.518(3)	0.024(8)
C3	0.762(6)	0.261(3)	0.528(3)	0.026(9)
C4	0.560(5)	0.087(3)	0.461(3)	0.017(6)
C5	0.497(4)	0.181(2)	0.517(2)	0.038(5)
N11	0.548(3)	0.2243(16)	0.6737(15)	0.027(4)
N12	0.599(5)	0.263(3)	0.765(3)	0.027(4)
N13	0.577(5)	0.979(3)	0.731(2)	0.021(6)
N14	0.553(5)	0.091(3)	0.6944(18)	0.023(6)
N15	0.617(5)	0.067(3)	0.7988(16)	0.022(5)
C11	0.563(5)	0.165(4)	0.707(3)	0.020(7)
C12	0.606(5)	0.174(4)	0.762(3)	0.021(8)
C13	0.565(6)	0.281(4)	0.710(4)	0.027(9)
C14	0.577(5)	0.063(3)	0.728(3)	0.019(6)

C15	0.627(5)	0.156(3)	0.813(3)	0.018(5)
N21	0.561(5)	0.352(3)	0.587(3)	0.022(6)
N22	0.418(5)	0.383(3)	0.527(3)	0.023(6)
N23	0.485(5)	0.104(3)	0.584(3)	0.033(9)
N24	0.361(6)	0.193(3)	0.533(3)	0.029(6)
N25	0.533(3)	0.2248(19)	0.5993(16)	0.045(6)
C21	0.506(7)	0.289(4)	0.583(3)	0.030(9)
C23	0.522(6)	0.395(4)	0.563(3)	0.024(6)
O1X	0.652(6)	0.325(4)	0.902(3)	0.21(2)
O2X	0.338(5)	0.448(3)	0.429(3)	0.19(2)
O11	0.661(4)	0.153(2)	0.862(2)	0.020(6)
C22	0.408(6)	0.307(4)	0.537(3)	0.024(5)
C24	0.320(6)	0.262(4)	0.515(4)	0.029(5)
O21	0.236(4)	0.268(2)	0.486(2)	0.026(10)
C1A	0.519(6)	0.125(3)	0.072(3)	0.070(11)
C2A	0.516(3)	0.0278(17)	0.0062(17)	0.065(7)
C3A	0.574(5)	0.085(3)	0.997(3)	0.046(7)
O1A	0.574(5)	0.085(3)	0.997(3)	0.046(7)
C4A	0.404(6)	0.005(2)	0.069(3)	0.078(11)
N1B	0.874(4)	0.113(2)	0.4363(19)	0.029(6)
N2B	0.866(3)	0.011(3)	0.492(2)	0.052(8)
N3B	0.055(4)	0.083(3)	0.455(2)	0.046(8)
N4B	0.257(3)	0.0607(18)	0.4790(15)	0.013(6)
C1B	0.981(3)	0.091(2)	0.4561(19)	0.039(5)
O1B	0.981(3)	0.091(2)	0.4561(19)	0.039(5)
C2B	0.975(3)	0.0240(19)	0.4865(15)	0.060(7)
C3B	0.798(3)	0.080(3)	0.458(2)	0.039(7)

C4B	0.150(4)	0.046(3)	0.482(2)	0.034(10)
N1A	0.584(4)	0.134(3)	0.028(2)	0.046(8)
N2A	0.474(4)	0.057(3)	0.052(2)	0.077(10)
N3A	0.354(5)	0.017(3)	0.115(3)	0.081(13)
N4A	0.403(4)	0.937(2)	0.041(3)	0.076(13)

Table S11. Bond lengths (Å) for compound **3**.

W001-O012	1.71(2)	W001-O00I	1.877(19)
W001-O00E	1.88(2)	W001-O00J	1.92(2)
W001-O00Y	1.93(2)	W001-O00W	2.43(2)
W002-O015	1.71(2)	W002-O00H	1.92(2)
W002-O00K	1.91(2)	W002-O00F	1.89(2)
W002-O00O	1.93(2)	W002-O00Z	2.432(18)
W003-O018	1.69(2)	W003-O00J	1.91(2)
W003-O00G	1.88(2)	W003-O00Q	1.90(2)
W003-O013	1.92(2)	W003-O00W	2.427(18)
W004-O1	1.68(2)	W004-O00O	1.91(2)
W004-O00N	1.90(2)	W004-O00R	1.89(2)
W004-O00G	1.95(2)	W004-O00Z	2.46(2)
W005-O01C	1.70(2)	W005-O00R	1.91(2)
W005-O00U	1.923(19)	W005-O00K	1.91(2)
W005-O00M	1.89(2)	W005-O00Z	2.446(19)
W006-O01G	1.71(2)	W006-O013	1.89(2)
W006-O00Y	1.90(2)	W006-O00U	1.89(2)
W006-O00T	1.91(2)	W006-O00W	2.451(19)
W007-O01F	1.69(2)	W007-O00Q	1.92(2)
W007-O00N	1.90(2)	W007-O00X	1.93(2)

W007-O00V	1.95(3)	W007-O19	2.421(18)
W008-O010	1.69(2)	W008-O00E	1.90(2)
W008-O011	1.90(2)	W008-O00X	1.91(2)
W008-O01A	1.91(2)	W008-O19	2.45(2)
W009-O016	1.68(2)	W009-O00V	1.91(2)
W009-O01A	1.92(2)	W009-O00F	1.92(2)
W009-O00S	1.91(2)	W009-O19	2.452(19)
W00A-O01H	1.71(2)	W00A-O011	1.89(2)
W00A-O017	1.90(2)	W00A-O00I	1.922(19)
W00A-O00L	1.91(3)	W00A-O00P	2.46(2)
W00B-O01I	1.70(2)	W00B-O00S	1.92(3)
W00B-O017	1.93(3)	W00B-O00H	1.88(2)
W00B-O014	1.94(3)	W00B-O00P	2.469(17)
W00C-O01E	1.71(2)	W00C-O014	1.89(2)
W00C-O00T	1.88(2)	W00C-O00M	1.92(3)
W00C-O00L	1.94(3)	W00C-O00P	2.422(19)
P00D-O00P	1.513(18)	P00D-O00W	1.526(18)
P00D-O00Z	1.52(2)	P00D-O19	1.527(19)
O1Z-N24	1.00(7)	O1Z-C5	1.29(5)
O1Z-N25	1.49(5)	O1Z-N23	1.81(7)
N1-C1	1.34(9)	N1-C3	1.28(9)
N2-C2	1.36(9)	N2-C3	1.44(10)
N3-C4	1.52(8)	N4-C4	1.36(8)
N4-C5	1.49(6)	N5-C4	0.97(8)
N5-C1	1.33(8)	C1-C2	1.41(10)
C2-C5	1.40(8)	C5-N24	1.87(8)
N11-C11	1.35(7)	N11-C13	1.35(8)

N11-N25	1.70(5)	N12-C13	1.29(10)
N12-C12	1.68(9)	N13-C14	1.58(8)
N14-C14	0.93(7)	N14-C11	1.43(8)
N15-C14	1.61(7)	N15-C15	1.70(8)
C11-C12	1.27(10)	C12-C15	1.19(10)
C15-O11	1.12(8)	N21-C21	1.36(9)
N21-C23	1.03(9)	N22-C23	1.37(9)
N22-C22	1.45(9)	N24-C24	1.41(10)
N25-C21	1.29(8)	C21-C22	1.45(10)
C22-C24	1.39(10)	C24-O21	1.11(9)
C1A-N2A	1.437(10)	C1A-N1A	1.50(8)
C1A-C2A	2.400(10)	C2A-C2A#1	1.13(7)
C2A-N2A	1.435(10)	C2A-C3A	1.36(8)
C3A-N4A#1	1.06(8)	C3A-N1A	1.17(8)
C4A-N3A	1.40(4)	C4A-N2A	1.442(10)
C4A-N4A	1.443(10)	N1B-C3B	1.35(7)
N1B-C1B	1.38(6)	N2B-C2B	1.439(6)
N2B-C3B	1.64(6)	N2B-C4B#2	1.28(7)
N2B-C1B	2.395(10)	N3B-C1B	0.96(6)
N3B-C4B	1.38(7)	N4B-C4B	1.41(6)
C1B-C2B	1.46(4)	C1B-C3B	2.33(5)
C2B-C2B#2	1.19(6)	C2B-C4B#2	2.32(7)
C2B-C3B	2.395(10)		

Table S12. Bond angles (°) for compound 3.

O012-W001-O00I	101.9(10)	O012-W001-O00E	104.2(10)
O00I-W001-O00E	85.0(8)	O012-W001-O00J	103.3(10)

Supplementary Information

O00I-W001-O00J	154.8(9)	O00E-W001-O00J	88.3(9)
O012-W001-O00Y	102.2(10)	O00I-W001-O00Y	87.7(9)
O00E-W001-O00Y	153.5(9)	O00J-W001-O00Y	87.7(9)
O012-W001-O00W	172.2(9)	O00I-W001-O00W	83.1(8)
O00E-W001-O00W	82.1(8)	O00J-W001-O00W	71.9(7)
O00Y-W001-O00W	71.8(8)	O015-W002-O00H	102.5(9)
O015-W002-O00K	101.7(10)	O00H-W002-O00K	89.4(10)
O015-W002-O00F	103.2(10)	O00H-W002-O00F	86.2(9)
O00K-W002-O00F	155.1(8)	O015-W002-O00O	101.1(9)
O00H-W002-O00O	156.4(9)	O00K-W002-O00O	86.9(9)
O00F-W002-O00O	87.5(9)	O015-W002-O00Z	171.1(9)
O00H-W002-O00Z	83.9(8)	O00K-W002-O00Z	72.0(7)
O00F-W002-O00Z	83.2(8)	O00O-W002-O00Z	72.7(8)
O018-W003-O00J	100.3(10)	O018-W003-O00G	102.7(10)
O00J-W003-O00G	157.1(8)	O018-W003-O00Q	103.5(12)
O00J-W003-O00Q	87.0(9)	O00G-W003-O00Q	87.9(9)
O018-W003-O013	100.9(12)	O00J-W003-O013	86.8(9)
O00G-W003-O013	88.7(9)	O00Q-W003-O013	155.5(8)
O018-W003-O00W	169.5(11)	O00J-W003-O00W	72.1(7)
O00G-W003-O00W	85.2(8)	O00Q-W003-O00W	83.6(7)
O013-W003-O00W	71.9(7)	O1-W004-O00O	101.9(10)
O1-W004-O00N	103.4(10)	O00O-W004-O00N	88.1(9)
O1-W004-O00R	102.3(11)	O00O-W004-O00R	87.5(9)
O00N-W004-O00R	154.3(9)	O1-W004-O00G	101.8(10)
O00O-W004-O00G	156.3(9)	O00N-W004-O00G	86.0(9)
O00R-W004-O00G	88.0(9)	O1-W004-O00Z	171.3(9)
O00O-W004-O00Z	72.2(8)	O00N-W004-O00Z	83.1(7)

Supplementary Information

O00R-W004-O00Z	71.4(8)	O00G-W004-O00Z	84.3(8)
O01C-W005-O00R	104.5(12)	O01C-W005-O00U	102.6(10)
O00R-W005-O00U	88.7(10)	O01C-W005-O00K	102.3(10)
O00R-W005-O00K	86.1(9)	O00U-W005-O00K	155.1(9)
O01C-W005-O00M	101.1(12)	O00R-W005-O00M	154.4(9)
O00U-W005-O00M	84.5(9)	O00K-W005-O00M	89.7(9)
O01C-W005-O00Z	172.6(10)	O00R-W005-O00Z	71.5(8)
O00U-W005-O00Z	83.6(7)	O00K-W005-O00Z	71.6(8)
O00M-W005-O00Z	83.3(8)	O01G-W006-O013	103.7(12)
O01G-W006-O00Y	102.7(10)	O013-W006-O00Y	87.7(9)
O01G-W006-O00U	102.5(10)	O013-W006-O00U	88.8(10)
O00Y-W006-O00U	154.7(8)	O01G-W006-O00T	101.7(11)
O013-W006-O00T	154.7(9)	O00Y-W006-O00T	87.6(9)
O00U-W006-O00T	85.0(10)	O01G-W006-O00W	172.7(8)
O013-W006-O00W	71.8(8)	O00Y-W006-O00W	71.7(8)
O00U-W006-O00W	83.4(7)	O00T-W006-O00W	83.1(7)
O01F-W007-O00Q	101.8(13)	O01F-W007-O00N	103.6(10)
O00Q-W007-O00N	86.9(9)	O01F-W007-O00X	100.8(11)
O00Q-W007-O00X	86.4(10)	O00N-W007-O00X	155.5(9)
O01F-W007-O00V	102.8(13)	O00Q-W007-O00V	155.4(9)
O00N-W007-O00V	88.0(9)	O00X-W007-O00V	88.5(10)
O01F-W007-O19	172.1(10)	O00Q-W007-O19	82.8(7)
O00N-W007-O19	82.9(7)	O00X-W007-O19	72.9(8)
O00V-W007-O19	72.6(8)	O010-W008-O00E	104.1(11)
O010-W008-O011	102.1(12)	O00E-W008-O011	84.6(9)
O010-W008-O00X	102.6(11)	O00E-W008-O00X	88.4(10)
O011-W008-O00X	155.3(10)	O010-W008-O01A	102.1(11)

Supplementary Information

O00E-W008-O01A	153.7(9)	O011-W008-O01A	88.8(10)
O00X-W008-O01A	87.1(11)	O010-W008-O19	172.4(9)
O00E-W008-O19	81.8(8)	O011-W008-O19	83.1(8)
O00X-W008-O19	72.4(8)	O01A-W008-O19	72.2(8)
O016-W009-O00V	100.2(12)	O016-W009-O01A	103.2(11)
O00V-W009-O01A	86.0(10)	O016-W009-O00F	101.4(11)
O00V-W009-O00F	87.9(9)	O01A-W009-O00F	155.2(9)
O016-W009-O00S	102.9(12)	O00V-W009-O00S	156.8(9)
O01A-W009-O00S	89.9(11)	O00F-W009-O00S	86.3(10)
O016-W009-O19	171.3(11)	O00V-W009-O19	72.4(8)
O01A-W009-O19	72.1(8)	O00F-W009-O19	83.2(8)
O00S-W009-O19	84.6(8)	O01H-W00A-O011	103.1(13)
O01H-W00A-O017	101.3(11)	O011-W00A-O017	90.3(10)
O01H-W00A-O00I	103.2(11)	O011-W00A-O00I	85.4(9)
O017-W00A-O00I	155.5(10)	O01H-W00A-O00L	100.4(13)
O011-W00A-O00L	156.5(10)	O017-W00A-O00L	86.3(10)
O00I-W00A-O00L	88.1(8)	O01H-W00A-O00P	171.3(12)
O011-W00A-O00P	83.7(8)	O017-W00A-O00P	73.0(8)
O00I-W00A-O00P	82.6(8)	O00L-W00A-O00P	73.0(9)
O01I-W00B-O00S	103.4(14)	O01I-W00B-O017	101.2(13)
O00S-W00B-O017	87.6(11)	O01I-W00B-O00H	103.1(13)
O00S-W00B-O00H	86.3(10)	O017-W00B-O00H	155.6(9)
O01I-W00B-O014	102.2(14)	O00S-W00B-O014	154.4(9)
O017-W00B-O014	87.3(11)	O00H-W00B-O014	88.0(11)
O01I-W00B-O00P	170.8(10)	O00S-W00B-O00P	83.1(8)
O017-W00B-O00P	72.2(8)	O00H-W00B-O00P	83.6(8)
O014-W00B-O00P	71.5(8)	O01E-W00C-O014	103.0(11)

Supplementary Information

O01E-W00C-O00T	100.3(11)	O014-W00C-O00T	156.4(9)
O01E-W00C-O00M	101.0(13)	O014-W00C-O00M	87.6(10)
O00T-W00C-O00M	84.5(9)	O01E-W00C-O00L	102.7(14)
O014-W00C-O00L	88.3(11)	O00T-W00C-O00L	90.1(9)
O00M-W00C-O00L	156.3(8)	O01E-W00C-O00P	174.5(13)
O014-W00C-O00P	73.3(8)	O00T-W00C-O00P	83.7(7)
O00M-W00C-O00P	83.1(7)	O00L-W00C-O00P	73.3(8)
O00P-P00D-O00W	109.1(11)	O00P-P00D-O00Z	108.0(11)
O00W-P00D-O00Z	110.8(11)	O00P-P00D-O19	111.0(11)
O00W-P00D-O19	108.8(11)	O00Z-P00D-O19	109.1(11)
W008-O00E-W001	154.4(12)	W002-O00F-W009	151.0(11)
W003-O00G-W004	149.4(11)	W002-O00H-W00B	151.2(13)
W001-O00I-W00A	151.9(11)	W003-O00J-W001	126.5(10)
W002-O00K-W005	127.3(10)	W00C-O00L-W00A	124.7(11)
W00C-O00M-W005	152.2(10)	W004-O00N-W007	152.0(13)
W004-O00O-W002	126.1(11)	P00D-O00P-W00C	127.3(11)
P00D-O00P-W00B	126.4(11)	W00C-O00P-W00B	88.7(6)
P00D-O00P-W00A	125.2(11)	W00C-O00P-W00A	88.8(6)
W00B-O00P-W00A	88.1(6)	W007-O00Q-W003	149.6(11)
W005-O00R-W004	128.6(12)	W00B-O00S-W009	150.5(13)
W00C-O00T-W006	152.7(13)	W005-O00U-W006	152.2(13)
W009-O00V-W007	125.2(11)	P00D-O00W-W001	126.3(11)
P00D-O00W-W003	125.6(11)	W001-O00W-W003	89.4(6)
P00D-O00W-W006	125.8(10)	W001-O00W-W006	89.1(6)
W003-O00W-W006	88.8(6)	W008-O00X-W007	125.5(12)
W006-O00Y-W001	127.2(11)	P00D-O00Z-W005	126.1(10)
P00D-O00Z-W002	127.2(11)	W005-O00Z-W002	89.1(6)

Supplementary Information

P00D-O00Z-W004	125.1(10)	W005-O00Z-W004	88.4(6)
W002-O00Z-W004	88.8(6)	W008-O011-W00A	152.4(12)
W006-O013-W003	127.4(10)	W00C-O014-W00B	126.3(12)
W00A-O017-W00B	126.7(12)	W009-O01A-W008	127.1(11)
P00D-O19-W007	127.2(10)	P00D-O19-W008	125.6(11)
W007-O19-W008	88.9(6)	P00D-O19-W009	125.0(11)
W007-O19-W009	89.5(6)	W008-O19-W009	88.6(6)

N24-O1Z-C5	108.(5)	N24-O1Z-N25	147.(5)
C5-O1Z-N25	93.(3)	N24-O1Z-N23	114.(5)
C5-O1Z-N23	87.(3)	N25-O1Z-N23	91.(3)
C1-N1-C3	112.(6)	C2-N2-C3	106.(6)
C4-N4-C5	119.(5)	C4-N5-C1	125.(7)
N1-C1-C2	107.(6)	N1-C1-N5	139.(7)
C2-C1-N5	114.(6)	C1-C2-C5	126.(6)
C1-C2-N2	106.(6)	C5-C2-N2	127.(6)
N1-C3-N2	107.(6)	N5-C4-N4	131.(7)
N5-C4-N3	125.(7)	N4-C4-N3	104.(5)
O1Z-C5-C2	132.(5)	O1Z-C5-N4	116.(4)
C2-C5-N4	104.(4)	O1Z-C5-N24	31.(3)
C2-C5-N24	155.(4)	N4-C5-N24	101.(4)

C11-N11-C13	108.(5)	C11-N11-N25	124.(4)
C13-N11-N25	127.(4)	C13-N12-C12	103.(6)
C14-N14-C11	113.(7)	C14-N15-C15	104.(4)
N11-C11-C12	116.(6)	N11-C11-N14	134.(6)
C12-C11-N14	109.(6)	C15-C12-C11	153.(8)
C15-C12-N12	104.(6)	C11-C12-N12	99.(6)
N12-C13-N11	112.(6)	N14-C14-N15	141.(7)

N14-C14-N13	128.(7)	N15-C14-N13	90.(4)
O11-C15-C12	163.(8)	O11-C15-N15	99.(5)
C12-C15-N15	96.(5)	C21-N21-C23	119.(7)
C23-N22-C22	100.(6)	O1Z-N24-C24	115.(7)
O1Z-N24-C5	41.(4)	C24-N24-C5	110.(5)
C21-N25-N11	105.(4)	C21-N25-O1Z	96.(4)
N11-N25-O1Z	124.(3)	N21-C21-C22	100.(6)
N21-C21-N25	135.(7)	C22-C21-N25	123.(7)
N22-C23-N21	116.(7)	C24-C22-C21	125.(7)
C24-C22-N22	130.(7)	C21-C22-N22	105.(6)
O21-C24-C22	135.(8)	O21-C24-N24	119.(7)
C22-C24-N24	105.(7)	N2A-C1A-N1A	97.(3)
N2A-C1A-C2A	33.3(6)	N1A-C1A-C2A	63.(3)
C2A#1-C2A-N2A	112.(5)	C2A#1-C2A-C3A	150.(6)
N2A-C2A-C3A	98.(4)	C2A#1-C2A-C1A	145.(5)
N2A-C2A-C1A	33.3(6)	C3A-C2A-C1A	65.(4)
N4A#1-C3A-C2A	96.(5)	N4A#1-C3A-N1A	144.(8)
C2A-C3A-N1A	120.(7)	N3A-C4A-N2A	122.(3)
N3A-C4A-N4A	123.(3)	N2A-C4A-N4A	115.(5)
C3B-N1B-C1B	117.(4)	C2B-N2B-C3B	102.(3)
C2B-N2B-C4B#2	117.(5)	C3B-N2B-C4B#2	141.(4)
C2B-N2B-C1B	34.5(19)	C3B-N2B-C1B	68.(2)
C4B#2-N2B-C1B	152.(4)	C1B-N3B-C4B	144.(7)
N3B-C1B-C2B	93.(5)	N3B-C1B-N1B	158.(6)
C2B-C1B-N1B	105.(3)	N3B-C1B-N2B	127.(5)
C2B-C1B-N2B	33.9(8)	N1B-C1B-N2B	71.(3)
N3B-C1B-C3B	166.(5)	C2B-C1B-C3B	74.5(16)

N1B-C1B-C3B	31.(2)	N2B-C1B-C3B	40.5(18)
N2B-C2B-C1B	112.(3)	N2B-C2B-C2B#2	103.(5)
C1B-C2B-C2B#2	146.(4)	N2B-C2B-C4B#2	29.(3)
C1B-C2B-C4B#2	141.(3)	C2B#2-C2B-C4B#2	73.(4)
N2B-C2B-C3B	42.(2)	C1B-C2B-C3B	70.(2)
C2B#2-C2B-C3B	144.(4)	C4B#2-C2B-C3B	71.(2)
N1B-C3B-N2B	103.(2)	N1B-C3B-C1B	32.(2)
N2B-C3B-C1B	71.9(13)	N1B-C3B-C2B	67.(2)
N2B-C3B-C2B	36.0(5)	C1B-C3B-C2B	35.9(13)
N3B-C4B-N4B	128.(6)	N3B-C4B-N2B#2	114.(5)
N4B-C4B-N2B#2	117.(5)	N3B-C4B-C2B#2	81.(4)
N4B-C4B-C2B#2	151.(4)	N2B#2-C4B-C2B#2	33.(2)
C3A-N1A-C1A	111.(6)	C1A-N2A-C2A	113.4(11)
C1A-N2A-C4A	138.(5)	C2A-N2A-C4A	108.(4)
C3A#1-N4A-C4A	138.(6)		

Table S13. Anisotropic atomic displacement parameters (Å2) for compound **3**.

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W001	0.0320(6)	0.0351(6)	0.0362(6)	-0.0104(5)	0.0066(5)	0.0009(5)
W002	0.0386(6)	0.0398(6)	0.0310(6)	-0.0013(5)	0.0048(5)	0.0126(5)
W003	0.0415(7)	0.0292(6)	0.0691(9)	-0.0206(6)	0.0294(6)	-0.0071(5)
W004	0.0347(6)	0.0323(6)	0.0544(8)	-0.0127(5)	0.0188(6)	-0.0044(5)
W005	0.0410(7)	0.0261(6)	0.0533(8)	-0.0123(5)	-0.0113(6)	0.0053(5)
W006	0.0345(6)	0.0254(6)	0.0647(9)	-0.0123(6)	-0.0136(6)	0.0074(5)
W007	0.0534(8)	0.0630(8)	0.0261(6)	-0.0134(6)	0.0129(5)	-0.0272(6)

W008	0.0297(6)	0.0764(10)	0.0328(6)	0.0152(6)	0.0011(5)	-0.0127(6)
W009	0.0274(6)	0.0810(10)	0.0331(6)	0.0200(6)	0.0030(5)	-0.0001(6)
W00A	0.0563(8)	0.0632(8)	0.0317(6)	0.0177(6)	0.0220(6)	0.0315(7)
W00B	0.0744(10)	0.0648(9)	0.0357(7)	0.0192(6)	0.0274(7)	0.0487(8)
W00C	0.0962(12)	0.0378(7)	0.0236(6)	-0.0066(5)	-0.0039(6)	0.0312(7)
P00D	0.017(3)	0.030(3)	0.011(2)	-0.003(2)	0.0033(19)	0.009(2)
O00E	0.035(6)	0.053(8)	0.031(7)	-0.005(7)	0.009(5)	-0.006(5)
O00F	0.037(7)	0.060(8)	0.024(7)	0.015(6)	0.005(6)	0.005(6)
O00G	0.033(8)	0.036(5)	0.069(11)	-0.011(6)	0.021(7)	-0.002(5)
O00H	0.068(10)	0.049(8)	0.028(7)	0.007(7)	0.011(7)	0.025(7)
O00I	0.035(8)	0.047(7)	0.031(8)	-0.004(6)	0.005(6)	0.010(7)
O00J	0.036(8)	0.033(7)	0.060(8)	-0.025(6)	0.021(7)	-0.015(6)
O00K	0.057(7)	0.026(7)	0.043(8)	-0.015(6)	-0.001(6)	0.011(6)
O00L	0.091(9)	0.050(8)	0.028(7)	0.006(6)	0.018(6)	0.046(6)
O00M	0.061(9)	0.029(7)	0.032(7)	-0.015(6)	-0.015(6)	0.025(6)
O00N	0.042(7)	0.055(8)	0.036(8)	-0.007(7)	0.020(6)	-0.008(6)
O00O	0.042(8)	0.047(7)	0.036(8)	-0.002(6)	0.010(6)	0.008(6)
O00P	0.043(7)	0.042(7)	0.025(6)	-0.005(5)	0.012(4)	0.019(5)
O00Q	0.055(7)	0.043(8)	0.048(7)	-0.026(6)	0.023(6)	-0.017(6)
O00R	0.037(8)	0.035(8)	0.066(7)	-0.010(6)	0.007(6)	0.003(6)
O00S	0.047(9)	0.076(11)	0.043(6)	0.025(6)	0.021(5)	0.024(7)
O00T	0.057(9)	0.031(7)	0.043(8)	-0.010(7)	-0.009(6)	0.012(7)
O00U	0.027(8)	0.031(5)	0.067(11)	-0.011(6)	-0.010(6)	0.011(5)
O00V	0.042(8)	0.078(9)	0.029(7)	0.005(6)	0.003(6)	-0.022(6)
O00W	0.028(6)	0.032(6)	0.040(7)	-0.011(5)	0.007(4)	0.006(5)
O00X	0.054(9)	0.072(9)	0.033(7)	-0.002(7)	0.007(7)	-0.027(7)
O00Y	0.035(7)	0.039(7)	0.048(8)	-0.007(6)	-0.001(6)	0.008(6)

O00Z	0.032(6)	0.033(6)	0.032(6)	-0.006(5)	0.001(4)	0.003(4)
O010	0.036(9)	0.089(11)	0.049(11)	0.030(9)	-0.007(9)	-0.021(9)
O011	0.037(9)	0.072(11)	0.042(6)	0.017(6)	0.015(5)	0.016(6)
O012	0.050(12)	0.041(7)	0.052(12)	-0.004(7)	0.013(9)	-0.001(7)
O013	0.027(7)	0.030(8)	0.082(7)	-0.009(6)	0.013(5)	-0.001(6)
O014	0.099(8)	0.054(9)	0.028(7)	0.002(6)	0.022(6)	0.040(7)
O015	0.062(13)	0.049(7)	0.039(11)	0.008(7)	0.023(8)	0.019(7)
O016	0.037(8)	0.089(14)	0.053(11)	0.030(11)	-0.001(8)	0.001(8)
O017	0.071(10)	0.076(7)	0.041(9)	0.021(7)	0.034(8)	0.039(7)
O018	0.059(11)	0.038(9)	0.114(15)	-0.032(11)	0.059(11)	-0.017(9)
O01A	0.031(8)	0.087(7)	0.052(9)	0.028(7)	0.006(7)	-0.008(6)
O01C	0.061(10)	0.031(9)	0.082(13)	-0.012(10)	-0.020(8)	0.004(8)
O01E	0.145(19)	0.057(14)	0.023(7)	-0.007(7)	-0.010(8)	0.040(10)
O01F	0.099(17)	0.079(16)	0.036(7)	-0.019(8)	0.029(8)	-0.042(10)
O01G	0.047(8)	0.028(10)	0.093(12)	-0.006(9)	-0.022(9)	0.010(7)
O01H	0.065(12)	0.108(15)	0.059(11)	0.055(12)	0.038(10)	0.050(8)
O01I	0.132(17)	0.093(13)	0.070(14)	0.039(11)	0.062(11)	0.092(15)
O19	0.027(6)	0.056(7)	0.025(5)	0.000(5)	0.010(4)	-0.002(4)
O1	0.046(11)	0.048(11)	0.071(10)	-0.011(9)	0.031(10)	-0.007(8)
O1Z	0.033(9)	0.028(7)	0.044(10)	-0.018(7)	0.010(7)	0.007(6)
C25	0.033(9)	0.028(7)	0.044(10)	-0.018(7)	0.010(7)	0.007(6)
N1	0.025(6)	0.024(6)	0.025(6)	0.0000(10)	0.0064(19)	-0.0001(10)
N2	0.040(19)	0.004(16)	0.03(2)	-0.002(14)	0.007(18)	0.003(12)
N3	0.016(5)	0.015(5)	0.015(5)	0.0001(9)	0.0041(15)	0.0000(9)
N4	0.016(5)	0.015(5)	0.015(5)	0.0001(9)	0.0041(15)	0.0000(9)
N5	0.016(5)	0.016(5)	0.016(5)	0.0000(10)	0.0043(17)	0.0000(10)
C1	0.024(15)	0.015(15)	0.019(19)	-0.004(13)	-0.002(14)	0.001(11)

C2	0.033(14)	0.011(16)	0.03(2)	-0.003(14)	0.007(14)	-0.003(11)
C3	0.035(18)	0.008(17)	0.03(2)	0.007(14)	0.001(18)	-0.003(13)
C4	0.017(6)	0.017(6)	0.017(6)	0.0001(10)	0.0045(18)	0.0001(10)
C5	0.034(10)	0.036(11)	0.044(12)	-0.019(10)	0.012(10)	-0.001(8)
N11	0.024(12)	0.022(7)	0.034(7)	0.005(6)	0.008(9)	0.009(9)
N12	0.024(12)	0.022(7)	0.034(7)	0.005(6)	0.008(9)	0.009(9)
N13	0.021(7)	0.021(7)	0.021(7)	0.000(2)	0.006(3)	0.000(2)
N14	0.023(6)	0.023(6)	0.023(6)	0.0000(10)	0.0062(18)	0.0001(10)
N15	0.022(5)	0.022(5)	0.022(5)	-0.0001(10)	0.0059(17)	0.0000(10)
C11	0.015(19)	0.024(7)	0.022(8)	0.002(8)	0.009(16)	0.010(17)
C12	0.017(19)	0.024(9)	0.021(8)	0.002(7)	0.006(16)	-0.003(17)
C13	0.03(2)	0.025(10)	0.033(11)	0.005(9)	0.02(2)	0.01(2)
C14	0.019(6)	0.019(6)	0.019(6)	-0.0001(10)	0.0051(18)	0.0000(10)
C15	0.018(5)	0.019(5)	0.019(5)	0.0000(10)	0.0050(17)	0.0000(10)
N21	0.022(6)	0.022(6)	0.022(6)	-0.0001(10)	0.0058(17)	0.0000(10)
N22	0.023(6)	0.023(6)	0.023(6)	0.0000(10)	0.0061(17)	0.0000(10)
N23	0.02(2)	0.028(10)	0.05(2)	-0.016(13)	0.014(18)	0.012(12)
N24	0.034(9)	0.025(9)	0.029(17)	-0.003(11)	0.013(9)	0.005(8)
N25	0.064(14)	0.027(8)	0.028(8)	0.003(8)	-0.014(10)	0.002(9)
C21	0.036(16)	0.025(9)	0.022(15)	0.001(11)	-0.002(13)	-0.001(10)
C23	0.024(6)	0.024(6)	0.024(6)	0.0000(10)	0.0063(19)	0.0000(10)
O1X	0.21(2)	0.21(2)	0.21(2)	0.000(2)	0.057(7)	0.000(2)
O2X	0.19(2)	0.19(2)	0.19(2)	0.000(2)	0.050(6)	0.000(2)
O11	0.019(6)	0.020(6)	0.019(6)	0.000(2)	0.005(2)	0.000(2)
C22	0.024(5)	0.024(5)	0.024(5)	0.0000(10)	0.0065(17)	0.0001(10)
C24	0.029(5)	0.029(5)	0.029(6)	0.0000(10)	0.0077(17)	-0.0002(10)
O21	0.024(15)	0.016(19)	0.04(3)	0.004(17)	0.010(15)	-0.004(11)

C1A	0.06(3)	0.08(2)	0.07(3)	0.01(2)	0.03(2)	0.02(2)
C2A	0.054(17)	0.060(15)	0.065(17)	0.014(14)	-0.011(12)	0.005(14)
C3A	0.041(18)	0.032(15)	0.051(18)	-0.003(13)	-0.009(13)	0.021(14)
O1A	0.041(18)	0.032(15)	0.051(18)	-0.003(13)	-0.009(13)	0.021(14)
C4A	0.07(3)	0.08(2)	0.08(3)	0.00(2)	0.010(19)	0.01(2)
N1B	0.029(6)	0.029(6)	0.029(6)	-0.0002(10)	0.0077(18)	0.0001(10)
N2B	0.081(16)	0.045(16)	0.023(16)	0.004(12)	0.001(15)	0.003(14)
N3B	0.039(10)	0.064(19)	0.033(17)	-0.020(15)	0.008(13)	0.027(13)
N4B	0.014(6)	0.012(6)	0.012(6)	0.000(2)	0.004(3)	-0.001(2)
C1B	0.041(8)	0.050(12)	0.027(12)	-0.007(10)	0.010(10)	0.025(10)
O1B	0.041(8)	0.050(12)	0.027(12)	-0.007(10)	0.010(10)	0.025(10)
C2B	0.075(13)	0.059(14)	0.035(14)	0.005(11)	-0.001(13)	0.023(11)
C3B	0.045(11)	0.042(16)	0.030(16)	0.005(14)	0.008(13)	-0.009(12)
C4B	0.018(11)	0.06(3)	0.03(2)	-0.01(2)	0.008(16)	0.000(13)
N1A	0.041(19)	0.044(15)	0.05(2)	-0.009(15)	0.011(16)	0.035(13)
N2A	0.06(2)	0.09(2)	0.07(2)	0.019(17)	0.002(16)	0.011(17)
N3A	0.081(13)	0.081(13)	0.081(13)	0.000(2)	0.021(4)	0.000(2)
N4A	0.05(3)	0.08(2)	0.08(3)	0.00(2)	0.00(3)	0.03(2)

Table S14. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for compound **4**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)
W1	0.88733(2)	0.97895(2)	0.39909(2)	0.01480(7)
W2	0.79010(2)	0.85356(2)	0.25676(2)	0.01662(8)
W3	0.85977(2)	0.07312(2)	0.25418(2)	0.01691(7)
W4	0.97525(2)	0.09779(2)	0.12187(2)	0.01694(8)

P1	0.000000	0.000000	0.25813(11)	0.0060(4)
O12	0.0399(3)	0.1976(3)	0.1669(2)	0.0199(9)
O11	0.000000	0.000000	0.3311(4)	0.0164(14)
O10	0.8735(3)	0.0457(3)	0.3398(2)	0.0181(9)
O9	0.0681(3)	0.0859(3)	0.1136(2)	0.0202(9)
O8	0.8074(3)	0.9596(3)	0.2393(2)	0.0202(9)
O7	0.9516(3)	0.1786(3)	0.2688(2)	0.0210(9)
O13	0.9299(3)	0.9124(3)	0.4307(2)	0.0177(9)
O6	0.8835(3)	0.0918(3)	0.1653(2)	0.0205(9)
O5	0.8258(3)	0.8918(3)	0.3408(2)	0.0187(9)
O4	0.9346(3)	0.9169(3)	0.2335(2)	0.0146(8)
O3	0.9664(3)	0.1306(3)	0.0485(2)	0.0283(11)
O2	0.8158(3)	0.9611(3)	0.4555(2)	0.0226(10)
O1	0.6877(3)	0.7974(3)	0.2654(2)	0.0263(11)
O14	0.7811(3)	0.0908(3)	0.2615(2)	0.0271(11)
O1A	0.1111(4)	0.3257(4)	0.0600(3)	0.0499(16)
N3	0.2039(5)	0.3571(4)	0.1402(3)	0.0386(16)
C4	0.2655(5)	0.3518(5)	0.1685(4)	0.0349(18)
C3	0.1677(6)	0.3205(6)	0.0833(4)	0.043(2)
N2	0.2002(6)	0.2780(5)	0.0563(3)	0.0460(19)
C2	0.2993(6)	0.3130(5)	0.1366(4)	0.042(2)
N1	0.2924(6)	0.3852(5)	0.2264(4)	0.054(2)
C1	0.2640(7)	0.2741(6)	0.0794(5)	0.049(2)

Table S14. Bond lengths (Å) for compound **4**.

W1-O2	1.704(4)	W1-O10	1.888(4)

W1-O13#2	1.893(4)	W1-O5	1.918(4)
W1-O13	1.929(4)	W1-O11	2.435(4)
W2-O1	1.699(5)	W2-O5	1.898(4)
W2-O8	1.909(5)	W2-O7#1	1.917(5)
W2-O12#1	1.925(4)	W2-O4	2.436(4)
W3-O14	1.696(5)	W3-O8	1.898(5)
W3-O7	1.914(5)	W3-O6	1.908(5)
W3-O10	1.924(4)	W3-O4#2	2.445(4)
W4-O3	1.701(5)	W4-O9	1.897(4)
W4-O12	1.917(5)	W4-O9#1	1.912(4)
W4-O6	1.922(5)	W4-O4#2	2.442(4)
P1-O4	1.532(4)	P1-O4#1	1.532(4)
P1-O4#2	1.532(4)	P1-O11	1.531(8)
O1A-C3	1.229(11)	N3-C4	1.362(12)
N3-C3	1.380(11)	C4-N1	1.347(12)
C4-C2	1.371(13)	C3-N2	1.364(13)
N2-C1	1.342(14)	C2-C1	1.393(13)

Table S15. Bond angles (°) for compound **4**.

O2-W1-O10	103.0(2)	O2-W1-O13#2	104.0(2)
O10-W1-O13#2	90.33(19)	O2-W1-O5	101.0(2)
O10-W1-O5	86.06(19)	O13#2-W1-O5	154.99(19)
O2-W1-O13	100.7(2)	O10-W1-O13	155.97(19)
O13#2-W1-O13	87.6(3)	O5-W1-O13	85.80(19)
O2-W1-O11	171.4(2)	O10-W1-O11	84.88(18)
O13#2-W1-O11	72.23(16)	O5-W1-O11	82.80(17)
O13-W1-O11	71.69(16)	O1-W2-O5	102.7(2)

Supplementary Information

O1-W2-O8	102.9(2)	O5-W2-O8	86.21(19)
O1-W2-O7#1	101.5(2)	O5-W2-O7#1	89.4(2)
O8-W2-O7#1	155.55(19)	O1-W2-O12#1	101.5(2)
O5-W2-O12#1	155.80(19)	O8-W2-O12#1	87.9(2)
O7#1-W2-O12#1	86.3(2)	O1-W2-O4	171.0(2)
O5-W2-O4	.12(17)	O8-W2-O4	83.30(17)
O7#1-W2-O4	72.33(17)	O12#1-W2-O4	71.88(17)
O14-W3-O8	103.2(2)	O14-W3-O7	102.2(2)
O8-W3-O7	154.56(19)	O14-W3-O6	101.6(2)
O8-W3-O6	89.5(2)	O7-W3-O6	87.4(2)
O14-W3-O10	102.8(2)	O8-W3-O10	84.85(19)
O7-W3-O10	87.60(19)	O6-W3-O10	155.61(19)
O14-W3-O4#2	171.5(2)	O8-W3-O4#2	82.85(17)
O7-W3-O4#2	72.16(17)	O6-W3-O4#2	72.22(17)
O10-W3-O4#2	83.52(17)	O3-W4-O9	103.3(2)
O3-W4-O12	102.4(2)	O9-W4-O12	89.4(2)
O3-W4-O9#1	103.0(2)	O9-W4-O9#1	85.5(3)
O12-W4-O9#1	154.58(19)	O3-W4-O6	101.4(2)
O9-W4-O6	155.26(19)	O12-W4-O6	86.5(2)
O9#1-W4-O6	87.9(2)	O3-W4-O4#2	171.3(2)
O9-W4-O4#2	83.45(17)	O12-W4-O4#2	71.85(16)
O9#1-W4-O4#2	82.82(17)	O6-W4-O4#2	72.08(16)
O4-P1-O4#1	109.23(18)	O4-P1-O4#2	109.23(18)
O4#1-P1-O4#2	109.23(18)	O4-P1-O11	109.71(17)
O4#1-P1-O11	109.71(17)	O4#2-P1-O11	109.71(17)
W4-O12-W2#2	126.7(2)	P1-O11-W1	125.86(14)
P1-O11-W1#2	125.86(14)	W1-O11-W1#2	89.2(2)

P1-O11-W1#1	125.86(14)	W1-O11-W1#1	89.2(2)
W1#2-O11-W1#1	89.2(2)	W1-O10-W3	151.7(3)
W4-O9-W4#2	152.1(3)	W3-O8-W2	152.4(3)
W3-O7-W2#2	126.5(2)	W1#1-O13-W1	126.8(2)
W3-O6-W4	126.7(2)	W2-O5-W1	150.5(3)
P1-O4-W2	125.1(2)	P1-O4-W4#1	126.2(2)
W2-O4-W4#	189.49(14)	P1-O4-W3#1	126.3(2)
W2-O4-W3#	188.98(14)	W4#1-O4-W3#	188.93(14)
C4-N3-C3	124.8(8)	N1-C4-C2	121.6(9)
N1-C4-N3	119.7(8)	C2-C4-N3	118.6(8)
O1A-C3-N2	123.8(9)	O1A-C3-N3	122.7(9)
N2-C3-N3	113.5(9)	C1-N2-C3	124.9(8)
C4-C2-C1	118.3(10)	N2-C1-C2	119.5(9)

Table S16. Anisotropic atomic displacement parameters (Å2) for compound **4**.

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W1	0.01403(12)	0.01785(13)	0.01277(13)	0.00060(8)	0.00209(8)	0.00816(10)
W2	0.01207(12)	0.01657(13)	0.01747(13)	-0.00119(9)	-0.00124(8)	0.00434(10)
W3	0.01685(13)	0.02003(14)	0.01823(13)	0.00123(9)	0.00020(9)	0.01251(11)
W4	0.02122(14)	0.01833(13)	0.01343(13)	0.00262(8)	-0.00066(8)	0.01152(11)
P1	0.0051(7)	0.0051(7)	0.0077(10)	0.000000	0.000000	0.0026(3)
O12	0.025(2)	0.016(2)	0.016(2)	0.0042(16)	0.0011(17)	0.0086(19)
O11	0.016(2)	0.016(2)	0.017(3)	0.000000	0.000000	0.0080(11)
O10	0.021(2)	0.017(2)	0.017(2)	0.0012(16)	-0.0009(17)	0.0101(19)
O9	0.019(2)	0.022(2)	0.022(2)	0.0024(18)	0.0004(17)	0.013(2)

O8	0.023(2)	0.018(2)	0.020(2)	-0.0011(17)	-0.0047(17)	0.010(2)
O7	0.025(2)	0.021(2)	0.022(2)	0.0007(18)	0.0017(18)	0.014(2)
O13	0.019(2)	0.020(2)	0.016(2)	0.0035(16)	0.0032(16)	0.0114(19)
O6	0.021(2)	0.023(2)	0.019(2)	0.0013(17)	-0.0019(17)	0.012(2)
O5	0.020(2)	0.015(2)	0.018(2)	-0.0012(16)	-0.0003(17)	0.0062(18)
O4	0.017(2)	0.012(2)	0.016(2)	0.0001(15)	0.0001(16)	0.0076(17)
O3	0.038(3)	0.034(3)	0.018(2)	0.003(2)	-0.003(2)	0.022(3)
O2	0.020(2)	0.031(3)	0.018(2)	0.0002(18)	0.0053(17)	0.013(2)
O1	0.012(2)	0.026(3)	0.032(3)	0.000(2)	0.0000(19)	0.003(2)
O14	0.023(3)	0.041(3)	0.028(3)	-0.001(2)	-0.001(2)	0.024(2)
O1A	0.055(4)	0.054(4)	0.039(4)	0.001(3)	0.002(3)	0.026(4)
N3	0.046(4)	0.035(4)	0.028(3)	-0.007(3)	0.005(3)	0.014(3)
C4	0.031(4)	0.027(4)	0.034(4)	0.006(3)	0.006(3)	0.004(3)
C3	0.043(5)	0.043(5)	0.026(4)	0.008(3)	0.005(4)	0.009(4)
N2	0.068(6)	0.034(4)	0.027(3)	-0.006(3)	0.002(3)	0.018(4)
C2	0.041(5)	0.038(5)	0.037(4)	0.006(4)	0.008(4)	0.012(4)
N1	0.060(6)	0.037(4)	0.057(5)	0.002(4)	0.007(4)	0.018(4)
C1	0.067(7)	0.042(5)	0.036(5)	0.006(4)	0.012(4)	0.025(5)

Table S17. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å2) for compound **4**.

	x/a	y/b	z/c	U(eq)
H3A	0.1863	0.3854	0.1592	0.046000
H2B	0.3447	0.3126	0.1527	0.050000
H1A	0.2638	0.4076	0.2399	0.081000
H1B	0.2867	0.3470	0.2538	0.081000

H1C	0.3446	0.4232	0.2238	0.081000
H1Z	0.2844	0.2458	0.0574	0.059000

Table S18. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for compound **5**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)
W1	0.29548(5)	0.98570(4)	0.90341(3)	0.02286(11)
W1A	0.76685(5)	0.50302(4)	0.40430(2)	0.02083(11)
W2	0.10828(5)	0.74013(5)	0.93736(2)	0.02216(11)
W2A	0.76275(5)	0.13222(5)	0.43442(2)	0.02184(11)
W3A	0.56039(4)	0.26747(4)	0.43581(2)	0.01984(10)
W4A	0.53322(4)	0.39762(4)	0.32193(3)	0.02043(11)
W3	0.45726(5)	0.99614(4)	0.77357(3)	0.02273(11)
W5A	0.50648(5)	0.00947(4)	0.34298(3)	0.02150(11)
W6A	0.96830(4)	0.36661(5)	0.40230(2)	0.02222(11)
W4	0.32888(5)	0.62750(5)	0.93770(2)	0.02313(11)
W5	0.51341(5)	0.86973(5)	0.90002(3)	0.02316(11)
W7A	0.47519(4)	0.14006(5)	0.22954(2)	0.02215(11)
W8A	0.93231(5)	0.50751(5)	0.27645(3)	0.02335(12)
W6	0.06357(5)	0.85832(5)	0.82192(3)	0.02281(11)
W7	0.02138(5)	0.59786(5)	0.73347(3)	0.02328(11)
W9A	0.91133(5)	0.13011(5)	0.31744(3)	0.02457(12)
W8	0.42554(5)	0.76353(5)	0.69244(2)	0.02339(11)
W9	0.22539(5)	0.86500(5)	0.69207(2)	0.02253(11)
W10A	0.65441(5)	0.01190(5)	0.22599(3)	0.02468(12)
W11A	0.69875(5)	0.39962(5)	0.19453(2)	0.02442(12)

W10	0.47552(5)	0.63357(5)	0.81963(3)	0.02239(11)
W11	0.07255(5)	0.48238(4)	0.84867(3)	0.02361(12)
W12A	0.87904(5)	0.27298(5)	0.19151(3)	0.02562(12)
W12	0.21910(5)	0.49425(4)	0.73018(3)	0.02342(11)
Si1A	0.7207(3)	0.2615(3)	0.31490(14)	0.0110(5)
Si1	0.2679(3)	0.7426(3)	0.81562(15)	0.0119(6)
O4	0.9545(10)	0.8998(9)	0.8094(5)	0.035(3)
O41A	0.6757(8)	0.2162(9)	0.4542(4)	0.025(2)
O1A	0.7799(8)	0.0375(9)	0.2788(4)	0.027(2)
O2A	0.8698(8)	0.4383(8)	0.4241(4)	0.024(2)
O5	0.5222(8)	0.9412(8)	0.8313(4)	0.024(2)
O3A	0.9386(9)	0.2236(9)	0.2550(4)	0.029(2)
O6	0.3688(8)	0.0210(8)	0.8321(4)	0.027(2)
O7	0.4067(8)	0.9330(8)	0.9222(5)	0.027(2)
O8	0.4874(8)	0.7180(8)	0.7545(4)	0.026(2)
O4A	0.6381(8)	0.0345(8)	0.3886(4)	0.024(2)
O5A	0.8460(8)	0.5369(8)	0.3344(5)	0.026(2)
O6A	0.9842(8)	0.4410(9)	0.3336(4)	0.025(2)
O7A	0.4955(8)	0.1322(8)	0.3883(4)	0.0233(19)
O9	0.1467(8)	0.8981(8)	0.7566(4)	0.025(2)
O10	0.3075(8)	0.6201(8)	0.6914(4)	0.026(2)
O8A	0.7558(8)	0.1370(9)	0.1910(5)	0.031(2)
O9A	0.4669(8)	0.2538(8)	0.2836(4)	0.027(2)
O10A	0.5820(8)	0.2554(8)	0.1931(4)	0.024(2)
O11	0.3435(8)	0.5299(8)	0.7813(4)	0.026(2)
O11A	0.4766(7)	0.3289(8)	0.3912(4)	0.0215(19)
O12	0.1210(8)	0.7146(8)	0.6937(4)	0.024(2)

O12A	0.9971(11)	0.0606(11)	0.3051(6)	0.046(3)
O14A	0.4122(9)	0.9001(8)	0.3729(5)	0.032(2)
O13	0.2325(9)	0.7030(8)	0.9552(4)	0.025(2)
O15A	0.4834(9)	0.2394(9)	0.4948(5)	0.030(2)
O16A	0.8546(8)	0.0738(9)	0.3894(5)	0.028(2)
O14	0.0514(8)	0.6010(8)	0.8932(4)	0.027(2)
O17A	0.3595(9)	0.1132(9)	0.1881(5)	0.032(2)
O18A	0.4144(8)	0.0350(8)	0.2859(4)	0.024(2)
O15	0.0887(8)	0.5037(9)	0.6976(4)	0.025(2)
O16	0.5690(9)	0.7665(9)	0.8626(5)	0.029(2)
O17	0.5557(9)	0.1258(8)	0.7700(4)	0.029(2)
O18	0.0155(9)	0.7909(9)	0.8933(5)	0.029(2)
O19	0.3254(11)	0.5616(9)	0.9974(5)	0.039(3)
O19A	0.7892(8)	0.3362(9)	0.1523(4)	0.029(2)
O20A	0.6256(8)	0.4353(8)	0.2564(5)	0.030(2)
O20	0.2000(9)	0.8951(9)	0.9566(4)	0.030(2)
O21	0.0087(8)	0.7100(8)	0.7847(4)	0.026(2)
O21A	0.6644(8)	0.4166(8)	0.4573(4)	0.025(2)
O22	0.1639(8)	0.9875(8)	0.8655(5)	0.026(2)
O23	0.3397(10)	0.1137(8)	0.9404(5)	0.032(2)
O24	0.1291(9)	0.4126(7)	0.7897(4)	0.026(2)
O22A	0.0883(8)	0.4496(9)	0.4403(5)	0.032(2)
O25	0.0323(9)	0.7106(9)	0.9976(5)	0.031(2)
O26	0.3258(9)	0.8108(8)	0.6519(4)	0.026(2)
O23A	0.9532(10)	0.2526(11)	0.1354(5)	0.039(3)
O27	0.4540(9)	0.7633(9)	0.9559(4)	0.029(2)
O28	0.4231(8)	0.5747(8)	0.8907(4)	0.026(2)

O24A	0.6551(9)	0.4568(10)	0.1411(5)	0.036(3)
O29	0.9716(8)	0.4954(8)	0.7916(5)	0.028(2)
O30	0.3517(8)	0.9967(8)	0.7162(4)	0.026(2)
C02B	0.5343(13)	0.7453(11)	0.4158(7)	0.032(3)
O31	0.5028(10)	0.7443(10)	0.6371(5)	0.036(3)
O25A	0.8311(8)	0.5208(9)	0.2206(4)	0.027(2)
O26A	0.7854(8)	0.3342(8)	0.2629(4)	0.0204(18)
O32	0.9838(10)	0.3726(9)	0.8809(5)	0.036(3)
O33	0.5653(9)	0.5704(9)	0.8033(5)	0.032(2)
O27A	0.0158(8)	0.2615(9)	0.3620(4)	0.027(2)
O28A	0.7551(10)	0.0603(9)	0.4935(5)	0.035(3)
O29A	0.0412(9)	0.6323(10)	0.2747(5)	0.038(3)
O30A	0.5590(9)	0.9343(8)	0.2829(4)	0.025(2)
O34	0.6316(9)	0.9579(10)	0.9392(5)	0.035(3)
O31A	0.6396(8)	0.5170(8)	0.3672(4)	0.0226(19)
O32A	0.4336(9)	0.4504(9)	0.3088(5)	0.030(2)
O33A	0.8976(8)	0.2597(8)	0.4544(4)	0.027(2)
O35	0.9025(9)	0.5568(10)	0.6925(5)	0.035(3)
O36	0.5092(9)	0.9137(9)	0.7153(5)	0.029(2)
C2B	0.0857(16)	0.5171(14)	0.0747(8)	0.040(4)
O34A	0.5325(8)	0.0375(8)	0.1930(4)	0.026(2)
O35A	0.9761(8)	0.4214(9)	0.2185(4)	0.026(2)
O36A	0.8164(9)	0.6276(9)	0.4438(5)	0.034(3)
O37	0.2031(8)	0.5209(8)	0.8933(4)	0.026(2)
O38	0.1708(10)	0.9074(9)	0.6358(5)	0.035(3)
O37A	0.6659(7)	0.3322(7)	0.3539(4)	0.0150(16)
O39	0.2296(9)	0.3894(9)	0.6858(5)	0.036(3)

O5B	0.8672(10)	0.6047(11)	0.0958(5)	0.044(3)
O38A	0.6560(10)	0.9028(9)	0.1821(5)	0.037(3)
O39A	0.8079(7)	0.2318(8)	0.3540(4)	0.0202(18)
N3G	0.5856(13)	0.0221(14)	0.5904(7)	0.050(4)
O1	0.3226(7)	0.8150(8)	0.7625(4)	0.0221(19)
O2	0.2057(8)	0.8074(8)	0.8555(4)	0.0209(18)
O3	0.1776(7)	0.6225(7)	0.7904(4)	0.0165(16)
O40A	0.6246(8)	0.1485(7)	0.2890(4)	0.0199(18)
O140	0.3628(8)	0.7246(7)	0.8542(4)	0.0196(18)
N1G	0.2892(10)	0.0038(11)	0.5283(5)	0.026(2)
O1F	0.8726(11)	0.3081(10)	0.5839(5)	0.040(3)
O1G	0.3008(10)	0.1402(10)	0.5969(5)	0.040(3)
O4C	0.0386(12)	0.0588(10)	0.6754(6)	0.046(3)
N2G	0.4406(10)	0.0816(10)	0.5924(5)	0.026(2)
N2C	0.2208(11)	0.2373(10)	0.8486(6)	0.030(3)
O1E	0.4568(11)	0.6854(10)	0.3053(5)	0.043(3)
O3G	0.9539(11)	0.9650(11)	0.4595(6)	0.048(3)
N1F	0.7950(12)	0.4356(11)	0.5828(6)	0.031(3)
O4G	0.1164(11)	0.8670(9)	0.4988(6)	0.041(3)
O1C	0.0372(9)	0.1620(11)	0.8452(6)	0.046(3)
O5E	0.5982(11)	0.8115(9)	0.4633(5)	0.040(3)
N1C	0.1246(10)	0.1637(11)	0.7612(6)	0.031(3)
O2F	0.6248(10)	0.2168(9)	0.6662(5)	0.040(3)
O4F	0.6056(10)	0.3999(11)	0.5943(5)	0.038(3)
N1E	0.6089(12)	0.7512(11)	0.3670(6)	0.033(3)
O3C	0.7988(11)	0.0064(12)	0.6704(6)	0.058(4)
O2D	0.4222(11)	0.3821(11)	0.9709(5)	0.045(3)

N2F	0.9822(14)	0.4827(13)	0.5656(7)	0.044(4)
O3F	0.5973(10)	0.3666(11)	0.7456(5)	0.040(3)
C8F	0.5566(12)	0.4003(13)	0.6483(7)	0.030(3)
C1E	0.5544(17)	0.7176(12)	0.3131(8)	0.039(4)
C7F	0.6420(12)	0.4056(11)	0.6925(6)	0.026(3)
O1X	0.7894(18)	0.6269(17)	0.8390(9)	0.099(7)
C1F	0.8821(13)	0.4043(13)	0.5786(7)	0.029(3)
N3B	0.0240(14)	0.5647(13)	0.0968(7)	0.044(4)
N3C	0.4116(13)	0.3181(13)	0.8525(7)	0.048(4)
C4C	0.3228(14)	0.2337(14)	0.7642(7)	0.036(4)
O4B	0.7041(11)	0.3216(9)	0.9996(5)	0.044(3)
C2G	0.4935(14)	0.0199(15)	0.5685(7)	0.034(3)
C7C	0.9463(13)	0.1697(14)	0.7221(7)	0.032(3)
O2C	0.8656(12)	0.1537(12)	0.7634(6)	0.054(4)
O2X	0.7778(10)	0.3151(11)	0.7913(6)	0.046(3)
C1G	0.3400(13)	0.0796(11)	0.5745(6)	0.027(3)
O2E	0.3752(12)	0.6150(15)	0.4571(7)	0.069(5)
C3B	0.9156(16)	0.5503(13)	0.0766(7)	0.038(4)
N2A	0.4895(16)	0.9473(13)	0.0694(7)	0.049(4)
C4F	0.8140(15)	0.5443(14)	0.5752(7)	0.036(4)
O4E	0.7371(13)	0.8988(11)	0.5632(6)	0.055(4)
C6F	0.6932(14)	0.3323(12)	0.6624(6)	0.030(3)
N3E	0.6247(15)	0.7202(13)	0.2675(7)	0.048(4)
C6G	0.1536(13)	0.0349(12)	0.4561(7)	0.032(3)
O5C	0.0122(14)	0.1843(13)	0.5438(6)	0.059(4)
O2G	0.1552(10)	0.1390(10)	0.4675(6)	0.049(4)
C5F	0.6883(13)	0.3550(14)	0.5994(7)	0.031(3)

O2B	0.6414(11)	0.5255(12)	0.9846(7)	0.061(4)
N1D	0.1816(15)	0.3856(15)	0.2790(7)	0.058(5)
C5C	0.1212(14)	0.1841(13)	0.8194(7)	0.032(3)
N1A	0.6306(16)	0.1100(16)	0.0492(8)	0.064(6)
O5F	0.6071(12)	0.5965(12)	0.6534(6)	0.055(4)
C10C	0.0609(14)	0.1948(15)	0.5995(8)	0.040(4)
O3AX	0.1413(12)	0.7386(10)	0.1756(6)	0.054(4)
O1D	0.1995(11)	0.2655(13)	0.9747(6)	0.056(4)
C6E	0.5644(15)	0.6323(14)	0.4816(7)	0.037(4)
O3B	0.6496(11)	0.4326(11)	0.8740(7)	0.058(4)
O3X	0.2362(13)	0.2425(17)	0.3543(8)	0.084(6)
C3C	0.3221(14)	0.2634(15)	0.8207(8)	0.037(4)
O6X	0.7559(14)	0.7334(14)	0.7419(7)	0.014(4)
C10B	0.7138(14)	0.4174(14)	0.9167(7)	0.037(4)
N1B	0.8743(12)	0.4646(11)	0.0357(6)	0.036(3)
O4X	0.7285(11)	0.9127(13)	0.7687(8)	0.018(4)
C1A	0.3824(19)	0.8826(17)	0.0846(9)	0.051(5)
N3A	0.3080(16)	0.9375(13)	0.0854(7)	0.052(5)
N3F	0.1031(15)	0.6544(14)	0.5470(8)	0.055(5)
C6A	0.1896(15)	0.8529(13)	0.1691(8)	0.042(4)
C2F	0.0011(17)	0.5885(14)	0.5565(8)	0.042(4)
C6B	0.7541(14)	0.4367(14)	0.0195(8)	0.046(5)
C7G	0.0448(12)	0.9530(13)	0.4319(8)	0.035(4)
O5X	0.2478(12)	0.5928(15)	0.3492(8)	0.077(5)
C9F	0.5152(15)	0.4932(16)	0.6533(9)	0.044(4)
C4B	0.0407(18)	0.4380(16)	0.0265(8)	0.052(5)
C4G	0.3415(15)	0.9473(15)	0.4988(7)	0.038(4)

O3E	0.5189(15)	0.5512(14)	0.5216(8)	0.079(5)
O2AX	0.1279(14)	0.9260(13)	0.0904(6)	0.061(4)
C5E	0.4802(16)	0.6260(14)	0.4323(8)	0.040(4)
C5G	0.1694(12)	0.9843(12)	0.5119(7)	0.031(3)
O1AX	0.3589(13)	0.7882(12)	0.0980(7)	0.064(4)
C3E	0.7416(18)	0.7613(15)	0.2747(8)	0.044(4)
C8B	0.6494(13)	0.3061(13)	0.9416(7)	0.034(3)
C1D	0.2730(14)	0.3145(16)	0.1303(8)	0.040(4)
C3F	0.9098(16)	0.6209(13)	0.5618(8)	0.040(4)
C6C	0.0170(14)	0.0949(14)	0.7312(7)	0.037(4)
C4D	0.3732(14)	0.3582(13)	0.0241(7)	0.033(3)
C11B	0.7374(15)	0.5020(14)	0.9724(8)	0.039(4)
C1C	0.2263(14)	0.1861(14)	0.7353(8)	0.038(4)
C8D	0.2295(15)	0.4053(16)	0.2194(7)	0.041(4)
C2E	0.7903(19)	0.7961(15)	0.3291(10)	0.053(6)
C4E	0.7220(16)	0.7924(14)	0.3748(8)	0.041(4)
C8G	0.0495(16)	0.8443(15)	0.4463(9)	0.046(5)
C2A	0.522(2)	0.0583(16)	0.0598(8)	0.060(7)
C4A	0.330(2)	0.0446(19)	0.0718(8)	0.066(7)
C7A	0.115(2)	0.9081(17)	0.1900(9)	0.065(7)
C3G	0.4397(15)	0.9456(16)	0.5172(7)	0.041(4)
C5D	0.2574(13)	0.2967(14)	0.0236(7)	0.032(3)
C7D	0.2224(15)	0.2936(18)	0.1863(8)	0.048(5)
C6D	0.2100(14)	0.2770(15)	0.0759(9)	0.045(4)
C5B	0.9347(17)	0.4131(15)	0.0111(7)	0.043(4)
C9C	0.9787(15)	0.0832(16)	0.6269(9)	0.047(5)
C8C	0.8819(15)	0.1030(15)	0.6584(10)	0.052(5)

N2B	0.1829(15)	0.5461(15)	0.0997(8)	0.059(5)
C3D	0.4359(16)	0.3976(19)	0.0740(8)	0.052(5)
C8E	0.7088(18)	0.7921(15)	0.5401(8)	0.047(5)
C7E	0.5983(15)	0.7469(13)	0.5121(8)	0.036(4)
C3A	0.436(2)	0.1046(15)	0.0606(9)	0.070(8)
O1B	0.7525(14)	0.2094(11)	0.8978(7)	0.070(5)
N2E	0.7946(17)	0.7592(17)	0.2279(8)	0.072(6)
O4AX	0.0498(14)	0.8681(12)	0.2353(7)	0.068(5)
C12B	0.6457(17)	0.2067(13)	0.9105(8)	0.045(5)
C9G	0.123(3)	0.816(3)	0.3979(15)	0.109(11)
C5A	0.1948(18)	0.8701(18)	0.1039(8)	0.055(6)
C8A	0.043(2)	0.9041(17)	0.1362(10)	0.063(7)
C2D	0.3835(16)	0.3684(18)	0.1265(8)	0.049(5)
C9A	0.981(3)	0.981(2)	0.1308(13)	0.091(10)
O5AX	0.925(2)	0.963(2)	0.0862(12)	0.133(9)
O7X	0.8140(15)	0.0210(18)	0.8652(10)	0.108(8)
O8X	0.9199(14)	0.8210(14)	0.6590(8)	0.079(5)
O5G	0.127(3)	0.715(3)	0.4143(14)	0.189(14)
O9X	0.2083(15)	0.4958(16)	0.5683(9)	0.088(6)
O10X	0.200(2)	0.014(2)	0.3159(10)	0.117(8)
O11X	0.301(2)	0.367(2)	0.5023(10)	0.122(8)

Table S19. Bond lengths (Å) for compound **5**.

W1-O23	1.720(10)	W1-O7	1.899(11)
W1-O20	1.915(10)	W1-O6	1.937(10)
W1-O22	1.946(10)	W1-O2	2.375(10)
W1A-O36A	1.709(10)	W1A-O2A	1.920(10)

W1A-O21A	1.931(10)	W1A-O5A	1.939(11)
W1A-O31A	1.955(9)	W1A-O37A	2.350(8)
W2-O25	1.718(11)	W2-O14	1.911(10)
W2-O13	1.921(11)	W2-O18	1.926(10)
W2-O20	1.949(11)	W2-O2	2.356(9)
W2A-O28A	1.725(12)	W2A-O41A	1.902(11)
W2A-O4A	1.912(10)	W2A-O16A	1.936(11)
W2A-O33A	1.943(10)	W2A-O39A	2.336(9)
W3A-O15A	1.700(11)	W3A-O7A	1.917(9)
W3A-O41A	1.933(10)	W3A-O11A	1.937(10)
W3A-O21A	1.942(9)	W3A-O37A	2.394(8)
W4A-O32A	1.732(10)	W4A-O31A	1.900(9)
W4A-O9A	1.905(10)	W4A-O11A	1.939(10)
W4A-O20A	1.942(11)	W4A-O37A	2.357(9)
W3-O17	1.713(10)	W3-O6	1.892(11)
W3-O5	1.925(10)	W3-O30	1.931(10)
W3-O36	1.963(11)	W3-O1	2.359(9)
W5A-O14A	1.705(10)	W5A-O7A	1.918(10)
W5A-O18A	1.932(10)	W5A-O4A	1.932(10)
W5A-O30A	1.940(10)	W5A-O40A	2.363(9)
W6A-O22A	1.731(10)	W6A-O33A	1.905(11)
W6A-O27A	1.911(11)	W6A-O2A	1.917(10)
W6A-O6A	1.925(10)	W6A-O39A	2.386(9)
W4-O19	1.699(11)	W4-O13	1.908(10)
W4-O27	1.927(11)	W4-O28	1.942(10)
W4-O37	1.944(10)	W4-O140	2.378(9)
W5-O34	1.747(11)	W5-O5	1.914(10)

W5-O16	1.929(11)	W5-O7	1.934(11)
W5-O27	1.940(10)	W5-O140	2.346(9)
W7A-O17A	1.703(10)	W7A-O10A	1.896(10)
W7A-O9A	1.924(11)	W7A-O34A	1.929(10)
W7A-O18A	1.940(10)	W7A-O40A	2.363(9)
W8A-O29A	1.722(11)	W8A-O5A	1.884(11)
W8A-O6A	1.914(10)	W8A-O25A	1.927(10)
W8A-O35A	1.932(10)	W8A-O26A	2.357(9)
W6-O4	1.742(12)	W6-O9	1.879(10)
W6-O22	1.922(10)	W6-O21	1.938(10)
W6-O18	1.955(10)	W6-O2	2.357(9)
W7-O35	1.707(10)	W7-O21	1.889(11)
W7-O12	1.910(10)	W7-O15	1.924(10)
W7-O29	1.934(10)	W7-O3	2.343(9)
W9A-O12A	1.711(12)	W9A-O1A	1.870(10)
W9A-O3A	1.937(11)	W9A-O16A	1.937(11)
W9A-O27A	1.968(10)	W9A-O39A	2.360(9)
W8-O31	1.714(11)	W8-O36	1.893(11)
W8-O8	1.909(11)	W8-O26	1.923(10)
W8-O10	1.931(10)	W8-O1	2.352(10)
W9-O38	1.728(10)	W9-O30	1.930(11)
W9-O12	1.935(10)	W9-O26	1.936(10)
W9-O9	1.952(10)	W9-O1	2.363(10)
W10A-O38A	1.709(11)	W10A-O30A	1.911(10)
W10A-O34A	1.925(10)	W10A-O8A	1.926(11)
W10A-O1A	1.964(11)	W10A-O40A	2.388(9)
W11A-O24A	1.715(11)	W11A-O20A	1.872(11)

W11A-O25A	1.914(10)	W11A-O19A	1.929(10)
W11A-O10A	1.930(10)	W11A-O26A	2.358(9)
W10-O33	1.708(11)	W10-O11	1.916(10)
W10-O16	1.916(11)	W10-O28	1.917(10)
W10-O8	1.934(10)	W10-O140	2.341(9)
W11-O32	1.708(11)	W11-O37	1.878(10)
W11-O24	1.910(10)	W11-O14	1.920(11)
W11-O29	1.943(11)	W11-O3	2.378(9)
W12A-O23A	1.706(11)	W12A-O8A	1.900(11)
W12A-O35A	1.936(10)	W12A-O19A	1.943(10)
W12A-O3A	1.946(11)	W12A-O26A	2.353(10)
W12-O39	1.714(10)	W12-O11	1.907(10)
W12-O15	1.920(10)	W12-O10	1.923(10)
W12-O24	1.947(10)	W12-O3	2.342(9)
Si1A-O40A	1.612(10)	Si1A-O37A	1.613(9)
Si1A-O39A	1.640(10)	Si1A-O26A	1.644(10)
Si1-O1	1.631(10)	Si1-O140	1.634(10)
Si1-O3	1.636(9)	Si1-O2	1.638(10)
C02B-O5E	1.414(19)	C02B-N1E	1.50(2)
C02B-C5E	1.54(2)	C2B-N3B	1.29(2)
C2B-N2B	1.30(2)	C2B-C4B	1.44(3)
O5B-C3B	1.19(2)	N3G-C2G	1.30(2)
N1G-C4G	1.35(2)	N1G-C1G	1.393(19)
N1G-C5G	1.533(19)	O1F-C1F	1.241(19)
O1G-C1G	1.195(18)	O4C-C6C	1.43(2)
O4C-C9C	1.50(2)	N2G-C2G	1.35(2)
N2G-C1G	1.37(2)	N2C-C5C	1.37(2)

N2C-C3C	1.42(2)	O1E-C1E	1.19(2)
O3G-C7G	1.41(2)	N1F-C1F	1.35(2)
N1F-C4F	1.38(2)	N1F-C5F	1.47(2)
O4G-C5G	1.439(18)	O4G-C8G	1.46(2)
O1C-C5C	1.21(2)	O5E-C7E	1.48(2)
N1C-C5C	1.38(2)	N1C-C1C	1.40(2)
N1C-C6C	1.49(2)	O2F-C6F	1.452(18)
O4F-C5F	1.43(2)	O4F-C8F	1.428(19)
N1E-C4E	1.38(2)	N1E-C1E	1.41(2)
O3C-C8C	1.37(2)	O2D-C4D	1.41(2)
N2F-C2F	1.35(2)	N2F-C1F	1.38(2)
O3F-C7F	1.430(18)	C8F-C7F	1.50(2)
C8F-C9F	1.51(2)	C1E-N3E	1.41(2)
C7F-C6F	1.51(2)	N3B-C3B	1.43(3)
N3C-C3C	1.31(2)	C4C-C1C	1.33(2)
C4C-C3C	1.36(2)	O4B-C6B	1.441(19)
O4B-C8B	1.50(2)	C2G-C3G	1.48(2)
C7C-O2C	1.41(2)	C7C-C6C	1.61(2)
C7C-C8C	1.72(3)	O2E-C5E	1.46(2)
C3B-N1B	1.36(2)	N2A-C2A	1.39(2)
N2A-C1A	1.40(3)	C4F-C3F	1.33(3)
O4E-C8E	1.38(2)	C6F-C5F	1.54(2)
N3E-C3E	1.42(3)	C6G-O2G	1.37(2)
C6G-C7G	1.50(2)	C6G-C5G	1.57(2)
O5C-C10C	1.43(2)	O2B-C11B	1.43(2)
N1D-C8D	1.54(2)	N1A-C2A	1.36(3)
O5F-C9F	1.43(2)	C10C-C9C	1.64(3)

O3AX-C6A	1.41(2)	O1D-C5D	1.32(2)
C6E-O3E	1.44(2)	C6E-C7E	1.52(2)
C6E-C5E	1.57(2)	O3B-C10B	1.38(2)
C10B-C8B	1.55(2)	C10B-C11B	1.60(2)
N1B-C5B	1.33(2)	N1B-C6B	1.51(2)
C1A-O1AX	1.23(2)	C1A-N3A	1.42(3)
N3A-C4A	1.39(3)	N3A-C5A	1.50(2)
N3F-C2F	1.32(2)	C6A-C7A	1.49(3)
C6A-C5A	1.57(2)	C2F-C3F	1.42(3)
C6B-C11B	1.52(3)	C7G-C8G	1.52(2)
C4B-C5B	1.34(3)	C4G-C3G	1.36(2)
O2AX-C5A	1.39(3)	O2AX-C8A	1.52(3)
C3E-N2E	1.31(2)	C3E-C2E	1.39(3)
C8B-C12B	1.43(2)	C1D-C2D	1.36(2)
C1D-C6D	1.46(2)	C1D-C7D	1.48(2)
C4D-C3D	1.38(2)	C4D-C5D	1.42(2)
C8D-C7D	1.58(3)	C2E-C4E	1.39(3)
C8G-C9G	1.60(4)	C2A-C3A	1.47(4)
C4A-C3A	1.35(3)	C7A-O4AX	1.38(2)
C7A-C8A	1.56(3)	C5D-C6D	1.38(2)
C9C-C8C	1.57(3)	C3D-C2D	1.42(3)
C8E-C7E	1.47(3)	O1B-C12B	1.42(2)
C9G-O5G	1.43(4)	C8A-C9A	1.53(4)
C9A-O5AX	1.24(3)		

Table S20. Bond angles (°) for compound **5**.

O23-W1-O7	103.0(5)	O23-W1-O20	101.6(5)

O7-W1-O20	90.2(5)	O23-W1-O6	101.3(5)
O7-W1-O6	86.3(5)	O20-W1-O6	157.1(4)
O23-W1-O22	98.8(5)	O7-W1-O22	158.0(4)
O20-W1-O22	87.5(5)	O6-W1-O22	87.3(4)
O23-W1-O2	170.9(5)	O7-W1-O2	84.5(4)
O20-W1-O2	73.0(4)	O6-W1-O2	84.2(4)
O22-W1-O2	73.9(4)	O36A-W1A-O2A	102.6(5)
O36A-W1A-O21A	99.3(5)	O2A-W1A-O21A	89.9(4)
O36A-W1A-O5A	102.2(5)	O2A-W1A-O5A	86.3(4)
O21A-W1A-O5A	158.4(4)	O36A-W1A-O31A	98.5(5)
O2A-W1A-O31A	158.8(4)	O21A-W1A-O31A	86.6(4)
O5A-W1A-O31A	89.3(4)	O36A-W1A-O37A	169.2(4)
O2A-W1A-O37A	86.0(4)	O21A-W1A-O37A	74.0(3)
O5A-W1A-O37A	84.5(4)	O31A-W1A-O37A	72.9(3)
O25-W2-O14	101.5(5)	O25-W2-O13	102.6(5)
O14-W2-O13	85.8(4)	O25-W2-O18	99.5(5)
O14-W2-O18	90.0(5)	O13-W2-O18	157.8(4)
O25-W2-O20	100.5(5)	O14-W2-O20	158.0(4)
O13-W2-O20	89.1(4)	O18-W2-O20	86.7(5)
O25-W2-O2	170.4(4)	O14-W2-O2	85.3(4)
O13-W2-O2	84.5(4)	O18-W2-O2	73.5(4)
O20-W2-O2	72.9(4)	O28A-W2A-O41A	102.8(5)
O28A-W2A-O4A	102.0(5)	O41A-W2A-O4A	86.8(4)
O28A-W2A-O16A	98.1(5)	O41A-W2A-O16A	159.1(4)
O4A-W2A-O16A	88.4(4)	O28A-W2A-O33A	99.7(5)
O41A-W2A-O33A	90.9(4)	O4A-W2A-O33A	158.1(4)
O16A-W2A-O33A	86.1(4)	O28A-W2A-O39A	169.0(4)

O41A-W2A-O39A	86.0(4)	O4A-W2A-O39A	84.8(4)
O16A-W2A-O39A	73.4(4)	O33A-W2A-O39A	73.3(4)
O15A-W3A-O7A	102.0(5)	O15A-W3A-O41A	101.2(5)
O7A-W3A-O41A	86.2(4)	O15A-W3A-O11A	100.7(5)
O7A-W3A-O11A	88.4(4)	O41A-W3A-O11A	158.1(4)
O15A-W3A-O21A	101.4(5)	O7A-W3A-O21A	156.5(4)
O41A-W3A-O21A	88.0(4)	O11A-W3A-O21A	88.6(4)
O15A-W3A-O37A	171.7(4)	O7A-W3A-O37A	84.0(4)
O41A-W3A-O37A	84.7(4)	O11A-W3A-O37A	73.6(3)
O21A-W3A-O37A	72.8(4)	O32A-W4A-O31A	101.5(5)
O32A-W4A-O9A	100.7(5)	O31A-W4A-O9A	157.7(4)
O32A-W4A-O11A	98.9(5)	O31A-W4A-O11A	88.8(4)
O9A-W4A-O11A	86.4(4)	O32A-W4A-O20A	102.8(5)
O31A-W4A-O20A	90.2(4)	O9A-W4A-O20A	86.2(4)
O11A-W4A-O20A	158.1(4)	O32A-W4A-O37A	171.7(4)
O31A-W4A-O37A	73.7(4)	O9A-W4A-O37A	84.1(4)
O11A-W4A-O37A	74.4(3)	O20A-W4A-O37A	84.3(4)
O17-W3-O6	101.5(5)	O17-W3-O5	101.2(5)
O6-W3-O5	85.7(4)	O17-W3-O30	100.1(5)
O6-W3-O30	90.7(4)	O5-W3-O30	158.7(4)
O17-W3-O36	100.0(5)	O6-W3-O36	158.4(4)
O5-W3-O36	88.9(4)	O30-W3-O36	86.7(5)
O17-W3-O1	170.8(4)	O6-W3-O1	85.6(4)
O5-W3-O1	84.9(4)	O30-W3-O1	73.8(4)
O36-W3-O1	73.1(4)	O14A-W5A-O7A	102.0(5)
O14A-W5A-O18A	100.7(5)	O7A-W5A-O18A	87.2(4)
O14A-W5A-O4A	101.4(5)	O7A-W5A-O4A	86.5(4)

O18A-W5A-O4A	157.9(4)	O14A-W5A-O30A	100.8(5)
O7A-W5A-O30A	157.2(4)	O18A-W5A-O30A	88.0(4)
O4A-W5A-O30A	89.6(4)	O14A-W5A-O40A	171.8(4)
O7A-W5A-O40A	83.4(4)	O18A-W5A-O40A	73.2(4)
O4A-W5A-O40A	85.1(4)	O30A-W5A-O40A	73.9(4)
O22A-W6A-O33A	101.9(5)	O22A-W6A-O27A	101.1(5)
O33A-W6A-O27A	88.9(4)	O22A-W6A-O2A	101.7(5)
O33A-W6A-O2A	88.2(4)	O27A-W6A-O2A	157.2(4)
O22A-W6A-O6A	101.1(5)	O33A-W6A-O6A	156.9(4)
O27A-W6A-O6A	88.6(4)	O2A-W6A-O6A	85.4(4)
O22A-W6A-O39A	172.3(4)	O33A-W6A-O39A	72.7(4)
O27A-W6A-O39A	73.6(4)	O2A-W6A-O39A	83.9(4)
O6A-W6A-O39A	84.5(4)	O19-W4-O13	102.4(5)
O19-W4-O27	101.0(5)	O13-W4-O27	89.5(5)
O19-W4-O28	100.9(5)	O13-W4-O28	156.6(4)
O27-W4-O28	88.8(4)	O19-W4-O37	101.4(5)
O13-W4-O37	84.9(4)	O27-W4-O37	157.6(4)
O28-W4-O37	87.8(4)	O19-W4-O140	171.3(5)
O13-W4-O140	84.4(4)	O27-W4-O140	73.4(4)
O28-W4-O140	72.7(4)	O37-W4-O140	84.5(4)
O34-W5-O5	102.7(5)	O34-W5-O16	100.4(5)
O5-W5-O16	91.0(4)	O34-W5-O7	101.8(5)
O5-W5-O7	85.4(4)	O16-W5-O7	157.8(4)
O34-W5-O27	98.0(5)	O5-W5-O27	159.2(4)
O16-W5-O27	87.0(5)	O7-W5-O27	88.6(5)
O34-W5-O140	169.2(4)	O5-W5-O140	85.7(4)
O16-W5-O140	72.4(4)	O7-W5-O140	85.4(4)

O27-W5-O140	73.9(4)	O17A-W7A-O10A	101.9(5)
O17A-W7A-O9A	100.6(5)	O10A-W7A-O9A	86.3(4)
O17A-W7A-O34A	101.0(5)	O10A-W7A-O34A	89.3(4)
O9A-W7A-O34A	158.4(4)	O17A-W7A-O18A	99.9(5)
O10A-W7A-O18A	158.2(4)	O9A-W7A-O18A	88.6(4)
O34A-W7A-O18A	87.7(4)	O17A-W7A-O40A	171.3(4)
O10A-W7A-O40A	85.4(4)	O9A-W7A-O40A	84.4(4)
O34A-W7A-O40A	74.2(4)	O18A-W7A-O40A	73.0(4)
O29A-W8A-O5A	102.8(5)	O29A-W8A-O6A	101.5(5)
O5A-W8A-O6A	85.1(4)	O29A-W8A-O25A	101.2(5)
O5A-W8A-O25A	88.9(4)	O6A-W8A-O25A	157.3(4)
O29A-W8A-O35A	99.6(5)	O5A-W8A-O35A	157.6(4)
O6A-W8A-O35A	89.1(4)	O25A-W8A-O35A	88.1(4)
O29A-W8A-O26A	170.9(5)	O5A-W8A-O26A	84.5(4)
O6A-W8A-O26A	84.4(4)	O25A-W8A-O26A	73.2(4)
O35A-W8A-O26A	73.4(4)	O4-W6-O9	102.2(5)
O4-W6-O22	100.3(5)	O9-W6-O22	90.9(4)
O4-W6-O21	102.0(5)	O9-W6-O21	85.3(4)
O22-W6-O21	157.6(4)	O4-W6-O18	98.7(5)
O9-W6-O18	158.9(4)	O22-W6-O18	88.7(5)
O21-W6-O18	87.0(4)	O4-W6-O2	170.2(5)
O9-W6-O2	86.5(4)	O22-W6-O2	74.8(4)
O21-W6-O2	83.0(4)	O18-W6-O2	73.0(4)
O35-W7-O21	102.5(5)	O35-W7-O12	102.6(5)
O21-W7-O12	86.1(4)	O35-W7-O15	100.0(5)
O21-W7-O15	157.5(4)	O12-W7-O15	87.5(4)
O35-W7-O29	99.5(5)	O21-W7-O29	89.6(5)

O12-W7-O29	158.0(4)	O15-W7-O29	88.2(5)
O35-W7-O3	170.4(5)	O21-W7-O3	84.3(4)
O12-W7-O3	84.5(4)	O15-W7-O3	73.6(4)
O29-W7-O3	73.5(4)	O12A-W9A-O1A	103.1(6)
O12A-W9A-O3A	103.3(6)	O1A-W9A-O3A	87.9(5)
O12A-W9A-O16A	98.7(6)	O1A-W9A-O16A	91.1(4)
O3A-W9A-O16A	157.6(4)	O12A-W9A-O27A	98.6(6)
O1A-W9A-O27A	158.3(4)	O3A-W9A-O27A	85.4(4)
O16A-W9A-O27A	87.3(4)	O12A-W9A-O39A	168.2(5)
O1A-W9A-O39A	85.5(4)	O3A-W9A-O39A	84.9(4)
O16A-W9A-O39A	72.8(4)	O27A-W9A-O39A	73.3(4)
O31-W8-O36	99.5(5)	O31-W8-O8	101.6(5)
O36-W8-O8	91.2(4)	O31-W8-O26	99.8(5)
O36-W8-O26	87.9(4)	O8-W8-O26	158.4(4)
O31-W8-O10	101.9(5)	O36-W8-O10	158.7(4)
O8-W8-O10	85.4(4)	O26-W8-O10	87.6(4)
O31-W8-O1	171.3(5)	O36-W8-O1	74.4(4)
O8-W8-O1	84.9(4)	O26-W8-O1	74.1(4)
O10-W8-O1	84.3(4)	O38-W9-O30	101.9(5)
O38-W9-O12	101.0(5)	O30-W9-O12	157.1(4)
O38-W9-O26	100.1(5)	O30-W9-O26	87.7(4)
O12-W9-O26	89.3(4)	O38-W9-O9	102.3(5)
O30-W9-O9	88.7(4)	O12-W9-O9	85.5(4)
O26-W9-O9	157.6(4)	O38-W9-O1	172.2(5)
O30-W9-O1	73.7(4)	O12-W9-O1	83.7(4)
O26-W9-O1	73.6(4)	O9-W9-O1	84.1(4)
O38A-W10A-O30A	99.8(5)	O38A-W10A-O34A	101.5(5)

O30A-W10A-O34A	89.1(4)	O38A-W10A-O8A	102.8(5)
O30A-W10A-O8A	157.2(4)	O34A-W10A-O8A	89.7(4)
O38A-W10A-O1A	101.5(5)	O30A-W10A-O1A	88.1(4)
O34A-W10A-O1A	157.0(4)	O8A-W10A-O1A	84.3(4)
O38A-W10A-O40A	171.7(5)	O30A-W10A-O40A	73.7(4)
O34A-W10A-O40A	73.6(4)	O8A-W10A-O40A	84.1(4)
O1A-W10A-O40A	83.7(4)	O24A-W11A-O20A	100.7(6)
O24A-W11A-O25A	100.2(5)	O20A-W11A-O25A	89.3(4)
O24A-W11A-O19A	100.3(5)	O20A-W11A-O19A	158.9(5)
O25A-W11A-O19A	88.3(5)	O24A-W11A-O10A	101.8(5)
O20A-W11A-O10A	84.7(4)	O25A-W11A-O10A	157.9(4)
O19A-W11A-O10A	89.7(4)	O24A-W11A-O26A	171.4(4)
O20A-W11A-O26A	85.1(4)	O25A-W11A-O26A	73.4(4)
O19A-W11A-O26A	74.1(4)	O10A-W11A-O26A	84.9(4)
O33-W10-O11	100.3(5)	O33-W10-O16	102.1(5)
O11-W10-O16	157.5(4)	O33-W10-O28	100.6(5)
O11-W10-O28	89.9(4)	O16-W10-O28	87.8(4)
O33-W10-O8	101.4(5)	O11-W10-O8	85.2(4)
O16-W10-O8	88.6(4)	O28-W10-O8	157.9(4)
O33-W10-O140	172.5(5)	O11-W10-O140	85.2(4)
O16-W10-O140	72.7(4)	O28-W10-O140	74.0(4)
O8-W10-O140	84.1(4)	O32-W11-O37	102.1(5)
O32-W11-O24	102.4(5)	O37-W11-O24	91.1(5)
O32-W11-O14	100.0(5)	O37-W11-O14	85.5(4)
O24-W11-O14	157.6(4)	O32-W11-O29	99.4(5)
O37-W11-O29	158.2(4)	O24-W11-O29	87.8(5)
O14-W11-O29	87.3(4)	O32-W11-O3	170.8(4)

O37-W11-O3	86.3(4)	O24-W11-O3	73.3(4)
O14-W11-O3	84.4(4)	O29-W11-O3	72.6(4)
O23A-W12A-O8A	103.7(6)	O23A-W12A-O35A	98.7(5)
O8A-W12A-O35A	157.5(4)	O23A-W12A-O19A	98.9(5)
O8A-W12A-O19A	90.0(5)	O35A-W12A-O19A	88.2(5)
O23A-W12A-O3A	103.2(5)	O8A-W12A-O3A	86.4(5)
O35A-W12A-O3A	86.9(4)	O19A-W12A-O3A	157.9(4)
O23A-W12A-O26A	169.3(5)	O8A-W12A-O26A	84.6(4)
O35A-W12A-O26A	73.4(4)	O19A-W12A-O26A	74.0(4)
O3A-W12A-O26A	83.9(4)	O39-W12-O11	102.0(5)
O39-W12-O15	100.2(5)	O11-W12-O15	157.8(4)
O39-W12-O10	100.7(5)	O11-W12-O10	86.7(4)
O15-W12-O10	89.2(4)	O39-W12-O24	101.2(5)
O11-W12-O24	87.2(4)	O15-W12-O24	88.6(5)
O10-W12-O24	158.1(4)	O39-W12-O3	171.8(4)
O11-W12-O3	84.2(4)	O15-W12-O3	73.7(4)
O10-W12-O3	84.9(4)	O24-W12-O3	73.5(4)
O40A-Si1A-O37A	109.1(5)	O40A-Si1A-O39A	109.1(5)
O37A-Si1A-O39A	109.6(5)	O40A-Si1A-O26A	110.0(5)
O37A-Si1A-O26A	109.1(5)	O39A-Si1A-O26A	110.0(5)
O1-Si1-O140	110.7(5)	O1-Si1-O3	108.9(5)
O140-Si1-O3	109.4(5)	O1-Si1-O2	109.1(5)
O140-Si1-O2	109.2(5)	O3-Si1-O2	109.4(5)
W2A-O41A-W3A	150.6(6)	W9A-O1A-W10A	151.7(6)
W6A-O2A-W1A	150.5(6)	W5-O5-W3	151.4(6)
W9A-O3A-W12A	148.3(6)	W3-O6-W1	151.1(6)
W1-O7-W5	151.0(6)	W8-O8-W10	152.6(6)

W2A-O4A-W5A	150.0(6)	W8A-O5A-W1A	151.7(6)
W8A-O6A-W6A	152.9(6)	W3A-O7A-W5A	151.5(6)
W6-O9-W9	151.7(6)	W12-O10-W8	150.3(6)
W12A-O8A-W10A	153.9(6)	W4A-O9A-W7A	150.0(6)
W7A-O10A-W11A	151.9(6)	W12-O11-W10	151.7(6)
W3A-O11A-W4A	121.3(5)	W7-O12-W9	151.1(5)
W4-O13-W2	151.8(6)	W2A-O16A-W9A	121.7(5)
W2-O14-W11	151.2(6)	W5A-O18A-W7A	122.1(5)
W12-O15-W7	121.4(5)	W10-O16-W5	122.8(6)
W2-O18-W6	121.6(5)	W11A-O19A-W12A	120.7(5)
W11A-O20A-W4A	152.4(6)	W1-O20-W2	122.6(6)
W7-O21-W6	152.6(6)	W1A-O21A-W3A	122.0(5)
W6-O22-W1	.7(5)	W11-O24-W12	121.9(5)
W8-O26-W9	121.2(5)	W4-O27-W5	121.5(5)
W10-O28-W4	121.9(5)	W7-O29-W11	122.1(5)
W9-O30-W3	121.5(5)	O5E-C02B-N1E	108.7(13)
O5E-C02B-C5E	108.3(13)	N1E-C02B-C5E	110.4(13)
W11A-O25A-W8A	122.3(5)	Si1A-O26A-W12A	124.7(5)
Si1A-O26A-W8A	124.4(5)	W12A-O26A-W8A	91.6(3)
Si1A-O26A-W11A	124.0(5)	W12A-O26A-W11A	91.2(3)
W8A-O26A-W11A	91.1(3)	W6A-O27A-W9A	121.8(5)
W10A-O30A-W5A	122.0(5)	W4A-O31A-W1A	121.9(5)
W6A-O33A-W2A	122.7(5)	W8-O36-W3	121.4(5)
N3B-C2B-N2B	115.2(19)	N3B-C2B-C4B	117.4(19)
N2B-C2B-C4B	127.3(19)	W10A-O34A-W7A	121.9(5)
W8A-O35A-W12A	121.6(5)	W11-O37-W4	152.2(6)
Si1A-O37A-W1A	124.2(5)	Si1A-O37A-W4A	125.3(5)

W1A-O37A-W4A	91.4(3)	Si1A-O37A-W3A	124.0(4)
W1A-O37A-W3A	91.1(3)	W4A-O37A-W3A	90.6(3)
Si1A-O39A-W2A	125.1(5)	Si1A-O39A-W9A	123.4(5)
W2A-O39A-W9A	92.2(3)	Si1A-O39A-W6A	124.0(5)
W2A-O39A-W6A	91.3(3)	W9A-O39A-W6A	91.2(3)
Si1-O1-W8	124.0(5)	Si1-O1-W3	123.8(5)
W8-O1-W3	91.1(3)	Si1-O1-W9	125.8(5)
W8-O1-W9	91.0(3)	W3-O1-W9	91.0(3)
Si1-O2-W2	124.4(5)	Si1-O2-W6	124.1(5)
W2-O2-W6	91.9(3)	Si1-O2-W1	124.5(5)
W2-O2-W1	91.5(3)	W6-O2-W1	90.5(3)
Si1-O3-W12	124.6(5)	Si1-O3-W7	124.4(5)
W12-O3-W7	91.3(3)	Si1-O3-W11	123.7(5)
W12-O3-W11	91.2(3)	W7-O3-W11	91.8(3)
Si1A-O40A-W5A	125.4(5)	Si1A-O40A-W7A	124.3(5)
W5A-O40A-W7A	91.6(3)	Si1A-O40A-W10A	124.6(5)
W5A-O40A-W10A	90.3(3)	W7A-O40A-W10A	90.3(3)
Si1-O140-W10	124.1(5)	Si1-O140-W5	123.7(5)
W10-O140-W5	92.1(3)	Si1-O140-W4	124.7(5)
W10-O140-W4	91.3(3)	W5-O140-W4	91.2(3)
C4G-N1G-C1G	122.1(14)	C4G-N1G-C5G	120.0(13)
C1G-N1G-C5G	117.9(12)	C6C-O4C-C9C	115.9(14)
C2G-N2G-C1G	125.8(13)	C5C-N2C-C3C	121.4(14)
C1F-N1F-C4F	117.4(15)	C1F-N1F-C5F	118.6(14)
C4F-N1F-C5F	123.8(15)	C5G-O4G-C8G	109.6(12)
C02B-O5E-C7E	112.6(12)	C5C-N1C-C1C	120.2(14)
C5C-N1C-C6C	116.0(14)	C1C-N1C-C6C	122.4(14)

C5F-O4F-C8F	108.3(12)	C4E-N1E-C1E	123.4(16)		
C4E-N1E-C02B	121.8(14)	C1E-N1E-C02B	114.7(14)		
C2F-N2F-C1F	125.6(16)	O4F-C8F-C7F	106.5(12)		
O4F-C8F-C9F	108.5(14)	C7F-C8F-C9F	116.2(14)		
O1E-C1E-N1E	124.4(17)	O1E-C1E-N3E	121.2(18)		
N1E-C1E-N3E	114.4(17)	O3F-C7F-C8F	114.0(12)		
O3F-C7F-C6F	112.1(12)	C8F-C7F-C6F	100.6(12)		
O1F-C1F-N1F	122.0(15)	O1F-C1F-N2F	120.5(15)		
N1F-C1F-N2F	117.5(14)	C2B-N3B-C3B	126.4(17)		
C1C-C4C-C3C	118.4(17)	C6B-O4B-C8B	111.2(13)		
N3G-C2G-N2G	121.8(16)	N3G-C2G-C3G	121.1(16)		
N2G-C2G-C3G	117.1(14)	O2C-C7C-C6C	111.0(13)		
O2C-C7C-C8C	108.3(14)	C6C-C7C-C8C	97.0(12)		
O1G-C1G-N2G	121.5(14)	O1G-C1G-N1G	123.3(15)		
N2G-C1G-N1G	115.2(13)	O5B-C3B-N1B	125.2(19)		
O5B-C3B-N3B	122.8(16)	N1B-C3B-N3B	112.0(17)		
C2A-N2A-C1A	123.(2)	C3F-C4F-N1F	125.9(17)		
O2F-C6F-C7F	110.9(12)	O2F-C6F-C5F	106.9(13)		
C7F-C6F-C5F	103.3(13)	C1E-N3E-C3E	123.0(16)		
O2G-C6G-C7G	113.7(14)	O2G-C6G-C5G	111.5(13)		
C7G-C6G-C5G	102.6(12)	O4F-C5F-N1F	109.2(14)		
O4F-C5F-C6F	106.5(13)	N1F-C5F-C6F	111.0(13)		
O1C-C5C-N2C	119.0(16)	O1C-C5C-N1C	124.2(16)		
N2C-C5C-N1C	116.8(15)	O5C-C10C-C9C	102.6(14)		
O3E-C6E-C7E	109.5(15)	O3E-C6E-C5E	113.5(15)		
C7E-C6E-C5E	106.0(14)	N3C-C3C-C4C	123.9(18)		
N3C-C3C-N2C	115.9(17)	C4C-C3C-N2C	120.3(15)		

O3B-C10B-C8B	109.1(14)	O3B-C10B-C11B	115.4(15)
C8B-C10B-C11B	101.4(13)	C5B-N1B-C3B	123.3(17)
C5B-N1B-C6B	123.4(14)	C3B-N1B-C6B	113.3(16)
O1AX-C1A-N2A	121.(2)	O1AX-C1A-N3A	124.(2)
N2A-C1A-N3A	114.1(18)	C4A-N3A-C1A	127.0(19)
C4A-N3A-C5A	119.(2)	C1A-N3A-C5A	114.2(18)
O3AX-C6A-C7A	110.4(15)	O3AX-C6A-C5A	108.7(14)
C7A-C6A-C5A	102.9(18)	N3F-C2F-N2F	118.(2)
N3F-C2F-C3F	125.4(18)	N2F-C2F-C3F	116.5(17)
O4B-C6B-N1B	108.9(16)	O4B-C6B-C11B	107.3(14)
N1B-C6B-C11B	113.6(13)	O3G-C7G-C6G	112.6(15)
O3G-C7G-C8G	107.9(15)	C6G-C7G-C8G	102.2(13)
O5F-C9F-C8F	109.4(14)	C5B-C4B-C2B	117.(2)
N1G-C4G-C3G	122.6(16)	C5A-O2AX-C8A	105.5(16)
O2E-C5E-C02B	106.8(15)	O2E-C5E-C6E	108.7(15)
C02B-C5E-C6E	98.5(13)	O4G-C5G-N1G	104.8(12)
O4G-C5G-C6G	104.6(12)	N1G-C5G-C6G	115.2(12)
N2E-C3E-C2E	125.(2)	N2E-C3E-N3E	115.(2)
C2E-C3E-N3E	119.5(17)	C12B-C8B-O4B	111.5(14)
C12B-C8B-C10B	118.4(15)	O4B-C8B-C10B	102.6(12)
C2D-C1D-C6D	115.7(17)	C2D-C1D-C7D	120.8(18)
C6D-C1D-C7D	123.5(16)	C4F-C3F-C2F	117.0(15)
O4C-C6C-N1C	108.6(14)	O4C-C6C-C7C	106.0(13)
N1C-C6C-C7C	109.6(13)	C3D-C4D-O2D	120.4(16)
C3D-C4D-C5D	122.4(16)	O2D-C4D-C5D	117.2(15)
O2B-C11B-C6B	107.7(15)	O2B-C11B-C10B	109.9(15)
C6B-C11B-C10B	103.4(14)	C4C-C1C-N1C	122.5(17)

N1D-C8D-C7D	111.0(16)	C3E-C2E-C4E	118.(2)
N1E-C4E-C2E	121.2(18)	O4G-C8G-C7G	106.8(14)
O4G-C8G-C9G	104.8(18)	C7G-C8G-C9G	105.(2)
N1A-C2A-N2A	115.(2)	N1A-C2A-C3A	128.(2)
N2A-C2A-C3A	117.3(19)	C3A-C4A-N3A	116.(3)
O4AX-C7A-C6A	118.6(19)	O4AX-C7A-C8A	111.(2)
C6A-C7A-C8A	104.2(17)	C4G-C3G-C2G	116.4(15)
O1D-C5D-C6D	123.0(15)	O1D-C5D-C4D	120.3(15)
C6D-C5D-C4D	116.6(15)	C1D-C7D-C8D	110.3(17)
C5D-C6D-C1D	123.4(15)	N1B-C5B-C4B	122.5(17)
O4C-C9C-C8C	101.3(16)	O4C-C9C-C10C	109.3(13)
C8C-C9C-C10C	111.4(15)	O3C-C8C-C9C	112.6(17)
O3C-C8C-C7C	107.4(16)	C9C-C8C-C7C	101.5(14)
C4D-C3D-C2D	118.2(18)	O4E-C8E-C7E	112.5(16)
C8E-C7E-O5E	108.8(14)	C8E-C7E-C6E	115.7(14)
O5E-C7E-C6E	100.4(13)	C4A-C3A-C2A	122.(2)
O1B-C12B-C8B	112.4(14)	O5G-C9G-C8G	102.(3)
O2AX-C5A-N3A	106.1(18)	O2AX-C5A-C6A	109.9(18)
N3A-C5A-C6A	113.7(16)	O2AX-C8A-C9A	108.(2)
O2AX-C8A-C7A	101.2(18)	C9A-C8A-C7A	123.(2)
C1D-C2D-C3D	123.3(18)	O5AX-C9A-C8A	115.(3)

Table S21. Anisotropic atomic displacement parameters (Å2) for compound **5**.

The anisotropic atomic displacement factor exponent takes the form: -2π2[h2 a*2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W1	0.0290(3)	0.0178(2)	0.0198(3)	0.0002(2)	0.0030(2)	0.0069(2)

W1A	0.0213(2)	0.0181(2)	0.0206(3)	-0.00086(19)	-0.0001(2)	0.0051(2)
W2	0.0270(3)	0.0227(3)	0.0165(3)	0.0053(2)	0.0063(2)	0.0085(2)
W2A	0.0232(2)	0.0257(3)	0.0193(3)	0.0081(2)	0.0018(2)	0.0111(2)
W3A	0.0223(2)	0.0208(2)	0.0164(2)	0.00256(19)	0.00510(19)	0.0080(2)
W4A	0.0206(2)	0.0213(2)	0.0211(3)	0.0021(2)	-0.0005(2)	0.0099(2)
W3	0.0252(3)	0.0184(2)	0.0193(3)	0.0052(2)	0.0035(2)	0.0016(2)
W5A	0.0234(3)	0.0174(2)	0.0213(3)	0.0022(2)	0.0027(2)	0.0049(2)
W6A	0.0183(2)	0.0281(3)	0.0192(3)	0.0042(2)	-0.00162(19)	0.0072(2)
W4	0.0277(3)	0.0239(3)	0.0181(3)	0.0077(2)	0.0006(2)	0.0090(2)
W5	0.0243(3)	0.0211(2)	0.0203(3)	0.0013(2)	-0.0036(2)	0.0045(2)
W7A	0.0208(2)	0.0241(3)	0.0187(3)	-0.0014(2)	-0.0036(2)	0.0060(2)
W8A	0.0204(2)	0.0251(3)	0.0210(3)	0.0084(2)	0.0024(2)	0.0033(2)
W6	0.0251(3)	0.0245(3)	0.0213(3)	0.0056(2)	0.0026(2)	0.0115(2)
W7	0.0218(2)	0.0220(3)	0.0217(3)	0.0027(2)	-0.0036(2)	0.0033(2)
W9A	0.0251(3)	0.0314(3)	0.0233(3)	0.0034(2)	0.0029(2)	0.0173(2)
W8	0.0286(3)	0.0252(3)	0.0170(3)	0.0046(2)	0.0072(2)	0.0105(2)
W9	0.0263(3)	0.0239(3)	0.0171(3)	0.0075(2)	0.0012(2)	0.0082(2)
W10A	0.0288(3)	0.0241(3)	0.0213(3)	-0.0041(2)	0.0019(2)	0.0114(2)
W11A	0.0228(3)	0.0334(3)	0.0172(3)	0.0107(2)	0.0013(2)	0.0092(2)
W10	0.0240(3)	0.0232(3)	0.0212(3)	0.0029(2)	0.0014(2)	0.0103(2)
W11	0.0267(3)	0.0174(2)	0.0210(3)	0.0045(2)	0.0017(2)	0.0014(2)
W12A	0.0246(3)	0.0357(3)	0.0177(3)	0.0048(2)	0.0062(2)	0.0122(2)
W12	0.0287(3)	0.0187(2)	0.0200(3)	-0.0016(2)	-0.0005(2)	0.0064(2)
Si1A	0.0122(12)	0.0158(14)	0.0065(13)	0.0017(10)	0.0000(10)	0.0067(11)
Si1	0.0135(13)	0.0111(13)	0.0100(14)	0.0021(10)	0.0019(11)	0.0032(11)
O4	0.041(6)	0.034(6)	0.033(6)	0.004(5)	-0.008(5)	0.016(5)
O41A	0.024(5)	0.033(5)	0.017(5)	0.007(4)	0.001(4)	0.008(4)

O1A	0.027(5)	0.029(5)	0.022(5)	-0.001(4)	0.005(4)	0.006(4)
O2A	0.023(5)	0.022(5)	0.025(5)	0.001(4)	-0.002(4)	0.004(4)
O5	0.027(5)	0.026(5)	0.019(5)	0.006(4)	0.005(4)	0.010(4)
O3A	0.030(5)	0.039(6)	0.022(5)	0.003(4)	0.004(4)	0.018(5)
O6	0.029(5)	0.025(5)	0.020(5)	0.002(4)	0.002(4)	0.003(4)
O7	0.030(5)	0.016(4)	0.030(6)	0.000(4)	0.001(4)	0.004(4)
O8	0.025(5)	0.023(5)	0.026(5)	0.004(4)	0.006(4)	0.005(4)
O4A	0.023(4)	0.026(5)	0.025(5)	0.005(4)	0.011(4)	0.009(4)
O5A	0.026(5)	0.022(5)	0.030(5)	0.005(4)	-0.003(4)	0.008(4)
O6A	0.024(5)	0.034(5)	0.018(5)	0.008(4)	0.008(4)	0.010(4)
O7A	0.025(5)	0.022(4)	0.022(5)	0.002(4)	-0.002(4)	0.008(4)
O9	0.028(5)	0.024(5)	0.021(5)	0.006(4)	0.004(4)	0.008(4)
O10	0.026(5)	0.029(5)	0.020(5)	0.000(4)	0.000(4)	0.006(4)
O8A	0.026(5)	0.035(6)	0.032(6)	0.003(5)	0.003(4)	0.012(4)
O9A	0.031(5)	0.026(5)	0.024(5)	0.007(4)	-0.003(4)	0.010(4)
O10A	0.017(4)	0.035(5)	0.019(5)	0.008(4)	0.003(3)	0.009(4)
O11	0.030(5)	0.026(5)	0.022(5)	0.003(4)	0.004(4)	0.013(4)
O11A	0.018(4)	0.024(5)	0.020(5)	0.002(4)	0.002(3)	0.005(4)
O12	0.028(5)	0.024(5)	0.016(5)	0.000(4)	-0.001(4)	0.005(4)
O12A	0.047(7)	0.054(8)	0.055(9)	0.007(7)	-0.001(6)	0.039(7)
O14A	0.034(6)	0.025(5)	0.032(6)	0.005(4)	0.009(5)	0.006(4)
O13	0.036(5)	0.018(4)	0.021(5)	0.001(4)	0.004(4)	0.009(4)
O15A	0.029(5)	0.039(6)	0.023(5)	-0.003(5)	0.003(4)	0.015(5)
O16A	0.023(5)	0.032(5)	0.035(6)	0.013(5)	0.005(4)	0.015(4)
O14	0.030(5)	0.028(5)	0.019(5)	0.003(4)	0.003(4)	0.005(4)
O17A	0.040(6)	0.028(5)	0.025(5)	-0.007(4)	-0.013(5)	0.012(5)
O18A	0.021(4)	0.024(5)	0.024(5)	-0.002(4)	0.000(4)	0.007(4)

O15	0.032(5)	0.036(5)	0.011(4)	-0.001(4)	-0.003(4)	0.017(4)
O16	0.031(5)	0.032(6)	0.026(5)	0.007(4)	-0.002(4)	0.013(4)
O17	0.040(6)	0.020(5)	0.023(5)	0.002(4)	0.005(4)	0.005(4)
O18	0.034(5)	0.031(5)	0.028(6)	0.011(4)	0.009(4)	0.020(5)
O19	0.055(8)	0.032(6)	0.039(7)	0.018(5)	0.008(6)	0.025(6)
O19A	0.029(5)	0.039(6)	0.025(5)	0.009(5)	0.004(4)	0.019(5)
O20A	0.026(5)	0.028(5)	0.028(6)	0.004(4)	0.000(4)	0.002(4)
O20	0.036(6)	0.029(5)	0.021(5)	0.008(4)	0.007(4)	0.009(5)
O21	0.023(5)	0.031(5)	0.023(5)	0.003(4)	-0.003(4)	0.008(4)
O21A	0.026(5)	0.027(5)	0.017(5)	-0.002(4)	-0.002(4)	0.003(4)
O22	0.031(5)	0.019(4)	0.030(6)	0.005(4)	0.002(4)	0.010(4)
O23	0.048(7)	0.021(5)	0.023(5)	-0.002(4)	0.001(5)	0.012(5)
O24	0.035(5)	0.014(4)	0.023(5)	0.002(4)	0.006(4)	0.002(4)
O22A	0.020(5)	0.037(6)	0.031(6)	0.003(5)	-0.008(4)	0.001(4)
O25	0.034(6)	0.033(6)	0.027(6)	0.008(5)	0.009(5)	0.012(5)
O26	0.034(5)	0.030(5)	0.017(5)	-0.001(4)	-0.002(4)	0.016(4)
O23A	0.039(6)	0.062(8)	0.024(6)	0.010(5)	0.018(5)	0.026(6)
O27	0.035(6)	0.034(5)	0.015(5)	0.003(4)	0.003(4)	0.010(5)
O28	0.032(5)	0.027(5)	0.018(5)	0.005(4)	0.005(4)	0.010(4)
O24A	0.031(6)	0.050(7)	0.024(6)	0.019(5)	-0.002(4)	0.008(5)
O29	0.021(5)	0.018(4)	0.034(6)	0.004(4)	0.002(4)	-0.003(4)
O30	0.030(5)	0.030(5)	0.023(5)	0.012(4)	0.005(4)	0.013(4)
C02B	0.038(8)	0.019(6)	0.041(9)	-0.003(6)	0.000(7)	0.013(6)
O31	0.041(6)	0.040(6)	0.027(6)	0.008(5)	0.014(5)	0.016(5)
O25A	0.024(5)	0.034(5)	0.018(5)	0.007(4)	0.003(4)	0.006(4)
O26A	0.024(4)	0.021(4)	0.014(4)	0.005(3)	0.002(3)	0.006(4)
O32	0.043(7)	0.022(5)	0.035(6)	0.008(5)	0.003(5)	0.003(5)

O33	0.028(5)	0.033(6)	0.037(6)	0.004(5)	0.002(5)	0.012(5)
O27A	0.022(5)	0.037(6)	0.022(5)	0.007(4)	0.002(4)	0.011(4)
O28A	0.040(6)	0.032(6)	0.038(7)	0.008(5)	0.004(5)	0.019(5)
O29A	0.031(6)	0.038(6)	0.034(6)	0.016(5)	0.001(5)	-0.001(5)
O30A	0.035(5)	0.020(4)	0.016(5)	-0.003(4)	-0.004(4)	0.007(4)
O34	0.033(6)	0.039(6)	0.033(6)	0.003(5)	-0.009(5)	0.012(5)
O31A	0.025(5)	0.025(5)	0.019(5)	0.001(4)	-0.002(4)	0.012(4)
O32A	0.028(5)	0.041(6)	0.030(6)	0.001(5)	0.001(4)	0.023(5)
O33A	0.031(5)	0.031(5)	0.022(5)	0.000(4)	-0.009(4)	0.016(4)
O35	0.024(5)	0.040(6)	0.029(6)	0.002(5)	-0.007(4)	-0.001(5)
O36	0.031(5)	0.032(5)	0.028(6)	0.014(4)	0.013(4)	0.012(4)
C2B	0.048(10)	0.032(8)	0.045(11)	0.008(7)	0.008(8)	0.018(8)
O34A	0.026(5)	0.023(5)	0.028(5)	-0.002(4)	0.003(4)	0.007(4)
O35A	0.021(4)	0.038(6)	0.016(5)	0.001(4)	0.003(4)	0.009(4)
O36A	0.030(5)	0.029(5)	0.034(6)	-0.009(5)	-0.005(5)	0.005(5)
O37	0.033(5)	0.017(4)	0.024(5)	0.005(4)	-0.006(4)	0.006(4)
O38	0.050(7)	0.035(6)	0.022(5)	0.015(5)	-0.001(5)	0.016(5)
O37A	0.019(4)	0.013(4)	0.015(4)	0.004(3)	0.004(3)	0.007(3)
O39	0.039(6)	0.034(6)	0.027(6)	-0.021(5)	-0.005(5)	0.009(5)
O5B	0.043(7)	0.043(7)	0.032(7)	-0.004(6)	0.007(6)	0.001(6)
O38A	0.044(7)	0.029(6)	0.036(7)	-0.008(5)	-0.002(5)	0.015(5)
O39A	0.020(4)	0.026(5)	0.017(4)	0.006(4)	0.005(3)	0.011(4)
N3G	0.040(8)	0.065(11)	0.051(10)	0.000(9)	-0.014(7)	0.030(8)
O1	0.019(4)	0.021(4)	0.023(5)	0.005(4)	0.001(4)	0.003(4)
O2	0.023(4)	0.027(5)	0.019(5)	0.004(4)	0.005(4)	0.016(4)
O3	0.020(4)	0.016(4)	0.009(4)	0.000(3)	0.001(3)	0.003(3)
O40A	0.024(4)	0.017(4)	0.020(5)	0.000(3)	0.000(4)	0.010(4)

O140	0.023(4)	0.019(4)	0.016(4)	0.002(3)	0.006(3)	0.008(4)
N1G	0.027(6)	0.034(6)	0.023(6)	0.004(5)	0.001(5)	0.017(5)
O1F	0.052(7)	0.041(6)	0.039(7)	0.013(5)	0.017(6)	0.029(6)
O1G	0.039(6)	0.042(7)	0.041(7)	-0.003(6)	0.006(5)	0.020(6)
O4C	0.062(8)	0.036(6)	0.047(8)	0.003(6)	-0.010(7)	0.026(6)
N2G	0.027(6)	0.025(6)	0.025(6)	0.004(5)	-0.001(5)	0.010(5)
N2C	0.031(6)	0.029(6)	0.024(6)	-0.005(5)	-0.010(5)	0.003(5)
O1E	0.044(7)	0.038(7)	0.039(7)	0.008(6)	-0.008(6)	0.007(6)
O3G	0.034(6)	0.052(8)	0.056(9)	0.010(7)	0.010(6)	0.011(6)
N1F	0.045(7)	0.027(6)	0.023(6)	0.004(5)	0.005(5)	0.015(5)
O4G	0.053(7)	0.021(5)	0.047(8)	0.008(5)	-0.002(6)	0.010(5)
O1C	0.023(5)	0.048(7)	0.052(8)	-0.009(6)	0.004(5)	0.000(5)
O5E	0.069(9)	0.026(5)	0.028(6)	0.000(5)	-0.008(6)	0.024(6)
N1C	0.025(6)	0.033(7)	0.034(7)	0.001(6)	-0.002(5)	0.010(5)
O2F	0.046(7)	0.028(6)	0.037(7)	0.003(5)	0.006(6)	0.003(5)
O4F	0.048(7)	0.052(7)	0.021(6)	-0.003(5)	-0.009(5)	0.029(6)
N1E	0.056(9)	0.034(7)	0.022(6)	0.007(5)	0.003(6)	0.030(7)
O3C	0.046(8)	0.056(9)	0.051(9)	0.010(7)	0.005(7)	-0.005(7)
O2D	0.044(7)	0.050(7)	0.032(7)	0.007(6)	0.007(6)	0.007(6)
N2F	0.048(9)	0.043(9)	0.050(9)	0.029(7)	0.019(7)	0.022(7)
O3F	0.043(7)	0.060(8)	0.024(6)	0.007(5)	0.012(5)	0.028(6)
C8F	0.022(6)	0.032(8)	0.028(8)	0.004(6)	0.000(5)	0.003(6)
C1E	0.065(12)	0.015(6)	0.033(9)	0.010(6)	0.009(8)	0.011(7)
C7F	0.024(6)	0.020(6)	0.030(8)	-0.002(5)	0.001(5)	0.004(5)
O1X	0.097(7)	0.100(7)	0.100(7)	0.010(3)	0.003(3)	0.037(4)
C1F	0.036(8)	0.029(7)	0.025(7)	0.004(6)	0.005(6)	0.017(6)
N3B	0.050(9)	0.040(8)	0.031(8)	-0.003(6)	0.005(7)	0.006(7)

N3C	0.054(10)	0.041(8)	0.043(9)	0.009(7)	-0.003(8)	0.011(8)
C4C	0.038(8)	0.041(9)	0.034(9)	-0.004(7)	0.003(7)	0.020(7)
O4B	0.054(8)	0.021(5)	0.039(7)	0.007(5)	0.002(6)	-0.005(5)
C2G	0.035(8)	0.050(10)	0.026(8)	0.007(7)	0.002(6)	0.025(7)
C7C	0.034(8)	0.041(9)	0.029(8)	0.005(7)	-0.005(6)	0.021(7)
O2C	0.071(10)	0.070(9)	0.045(8)	0.014(7)	0.021(7)	0.051(8)
O2X	0.041(7)	0.046(7)	0.048(8)	0.004(6)	0.005(6)	0.011(6)
C1G	0.034(7)	0.016(6)	0.026(7)	-0.002(5)	0.009(6)	0.004(5)
O2E	0.042(8)	0.110(14)	0.053(10)	0.010(9)	0.010(7)	0.027(8)
C3B	0.054(10)	0.028(7)	0.020(7)	0.007(6)	0.012(7)	0.002(7)
N2A	0.072(11)	0.045(9)	0.025(7)	0.012(7)	0.019(7)	0.014(8)
C4F	0.045(9)	0.041(9)	0.027(8)	0.008(7)	-0.001(7)	0.023(8)
O4E	0.078(10)	0.041(7)	0.042(8)	0.003(6)	-0.005(7)	0.019(7)
C6F	0.040(8)	0.033(7)	0.020(7)	0.006(6)	0.014(6)	0.016(7)
N3E	0.072(12)	0.044(9)	0.029(8)	0.012(7)	0.007(8)	0.022(8)
C6G	0.032(7)	0.027(7)	0.027(8)	0.013(6)	0.000(6)	0.000(6)
O5C	0.083(11)	0.078(10)	0.028(7)	0.007(7)	-0.005(7)	0.044(9)
O2G	0.039(7)	0.044(7)	0.060(9)	0.032(7)	-0.003(6)	0.006(6)
C5F	0.032(7)	0.036(8)	0.026(8)	0.002(6)	0.000(6)	0.012(6)
O2B	0.038(7)	0.055(9)	0.082(12)	-0.020(8)	0.014(7)	0.014(7)
N1D	0.064(11)	0.070(12)	0.031(9)	0.021(8)	0.011(8)	0.012(9)
C5C	0.042(9)	0.028(7)	0.034(9)	0.005(6)	-0.003(7)	0.021(7)
N1A	0.070(13)	0.060(12)	0.044(11)	0.016(9)	0.002(9)	0.004(10)
O5F	0.068(10)	0.054(9)	0.052(9)	0.002(7)	0.009(7)	0.035(8)
C10C	0.030(8)	0.048(10)	0.043(10)	0.003(8)	0.002(7)	0.015(8)
O3AX	0.076(10)	0.027(6)	0.036(7)	-0.001(5)	0.007(7)	-0.007(6)
O1D	0.042(7)	0.092(12)	0.033(7)	-0.001(7)	0.008(6)	0.024(8)

C6E	0.047(9)	0.038(9)	0.028(8)	0.014(7)	0.005(7)	0.016(7)
O3B	0.049(8)	0.044(8)	0.073(11)	-0.007(7)	-0.029(8)	0.010(6)
O3X	0.040(8)	0.124(16)	0.080(13)	0.041(12)	0.015(8)	0.016(9)
C3C	0.033(8)	0.040(9)	0.035(9)	0.007(7)	-0.010(7)	0.009(7)
O6X	0.012(8)	0.018(9)	0.009(8)	-0.001(6)	0.002(6)	0.003(7)
C10B	0.038(9)	0.044(9)	0.031(9)	0.008(7)	0.005(7)	0.015(7)
N1B	0.045(8)	0.026(6)	0.024(7)	0.002(5)	0.003(6)	-0.003(6)
O4X	0.004(6)	0.018(8)	0.028(10)	0.000(7)	0.001(6)	0.001(6)
C1A	0.069(14)	0.040(10)	0.032(10)	-0.007(8)	0.004(9)	0.011(10)
N3A	0.068(12)	0.031(7)	0.035(8)	0.002(6)	0.016(8)	-0.007(7)
N3F	0.060(11)	0.051(10)	0.045(10)	0.010(8)	0.015(8)	0.010(9)
C6A	0.039(9)	0.028(8)	0.038(10)	-0.003(7)	0.003(7)	-0.010(7)
C2F	0.063(12)	0.030(8)	0.029(9)	0.004(7)	0.004(8)	0.012(8)
C6B	0.036(9)	0.034(8)	0.042(10)	-0.010(7)	0.023(8)	-0.013(7)
C7G	0.018(6)	0.031(8)	0.051(11)	-0.002(7)	-0.009(6)	0.005(6)
O5X	0.039(8)	0.098(14)	0.077(12)	-0.013(11)	-0.002(8)	0.011(8)
C9F	0.043(10)	0.054(11)	0.048(11)	0.011(9)	0.005(8)	0.032(9)
C4B	0.068(14)	0.045(11)	0.024(9)	-0.005(8)	-0.010(9)	0.004(10)
C4G	0.046(10)	0.045(10)	0.024(8)	-0.007(7)	0.004(7)	0.020(8)
O3E	0.080(6)	0.078(6)	0.076(6)	0.011(3)	0.001(3)	0.027(3)
O2AX	0.078(11)	0.058(9)	0.036(8)	0.007(7)	-0.005(8)	0.014(8)
C5E	0.051(10)	0.036(9)	0.035(9)	0.007(7)	0.004(8)	0.019(8)
C5G	0.028(7)	0.028(7)	0.032(8)	0.000(6)	-0.002(6)	0.005(6)
O1AX	0.073(11)	0.041(8)	0.056(10)	0.006(7)	0.008(8)	-0.002(7)
C3E	0.068(13)	0.039(9)	0.031(9)	0.016(7)	0.017(9)	0.024(9)
C8B	0.024(7)	0.031(8)	0.041(9)	0.009(7)	0.003(6)	0.005(6)
C1D	0.030(8)	0.056(11)	0.039(10)	0.018(8)	0.010(7)	0.020(8)

C3F	0.063(12)	0.023(7)	0.038(10)	0.006(7)	0.002(8)	0.020(8)
C6C	0.037(8)	0.038(9)	0.033(9)	-0.009(7)	-0.006(7)	0.014(7)
C4D	0.049(9)	0.028(7)	0.031(8)	0.003(6)	0.011(7)	0.025(7)
C11B	0.039(9)	0.032(8)	0.039(10)	-0.007(7)	0.008(7)	0.006(7)
C1C	0.034(8)	0.041(9)	0.036(9)	0.019(7)	0.008(7)	0.011(7)
C8D	0.038(9)	0.062(12)	0.027(8)	0.005(8)	0.009(7)	0.025(9)
C2E	0.059(13)	0.032(9)	0.064(14)	0.011(9)	0.027(11)	0.010(9)
C4E	0.051(11)	0.034(9)	0.039(10)	0.007(7)	-0.009(8)	0.015(8)
C8G	0.042(10)	0.037(9)	0.054(12)	-0.004(8)	-0.022(9)	0.010(8)
C2A	0.089(17)	0.030(9)	0.031(10)	-0.004(7)	0.010(11)	-0.010(10)
C4A	0.072(15)	0.061(14)	0.031(10)	-0.004(10)	0.018(10)	-0.012(12)
C7A	0.10(2)	0.036(10)	0.041(12)	0.003(9)	0.029(12)	0.011(11)
C3G	0.047(10)	0.053(11)	0.031(9)	-0.010(8)	0.001(7)	0.032(9)
C5D	0.028(7)	0.042(9)	0.026(8)	-0.001(7)	0.003(6)	0.016(7)
C7D	0.032(8)	0.073(14)	0.040(10)	0.009(10)	0.009(8)	0.020(9)
C6D	0.025(7)	0.046(10)	0.057(12)	-0.001(9)	-0.004(8)	0.009(7)
C5B	0.069(13)	0.039(9)	0.018(8)	-0.002(7)	-0.003(8)	0.019(9)
C9C	0.035(9)	0.051(11)	0.053(12)	-0.024(9)	-0.010(8)	0.019(8)
C8C	0.041(10)	0.043(10)	0.076(15)	0.022(10)	0.007(10)	0.018(8)
N2B	0.054(11)	0.058(11)	0.061(12)	0.000(9)	-0.003(9)	0.017(9)
C3D	0.034(9)	0.086(16)	0.029(9)	-0.007(10)	-0.001(7)	0.019(10)
C8E	0.080(14)	0.045(10)	0.028(9)	-0.004(8)	-0.004(9)	0.039(10)
C7E	0.047(9)	0.031(8)	0.038(9)	0.006(7)	0.010(8)	0.022(7)
C3A	0.12(2)	0.020(8)	0.049(12)	0.024(8)	0.021(13)	0.005(11)
O1B	0.089(12)	0.033(7)	0.086(13)	-0.005(8)	0.034(10)	0.022(8)
N2E	0.087(15)	0.081(14)	0.070(14)	0.034(11)	0.053(12)	0.051(12)
O4AX	0.081(12)	0.056(9)	0.061(10)	0.018(8)	0.029(9)	0.018(8)

C12B	0.065(13)	0.024(8)	0.032(9)	-0.012(7)	-0.002(9)	0.005(8)
C9G	0.110(11)	0.109(11)	0.109(11)	0.0093(17)	0.0037(15)	0.042(4)
C5A	0.061(13)	0.055(12)	0.018(8)	-0.005(8)	0.007(8)	-0.011(10)
C8A	0.076(16)	0.036(10)	0.051(13)	-0.007(9)	0.001(12)	-0.006(10)
C2D	0.043(10)	0.076(14)	0.039(10)	0.008(10)	-0.007(8)	0.035(10)
C9A	0.09(2)	0.09(2)	0.09(2)	-0.013(18)	-0.034(18)	0.037(18)
O5AX	0.133(9)	0.133(9)	0.134(9)	0.012(3)	0.005(3)	0.052(4)
O7X	0.053(11)	0.119(17)	0.15(2)	0.012(15)	0.052(12)	0.031(11)
O8X	0.068(11)	0.069(11)	0.097(15)	0.000(10)	0.009(11)	0.025(9)
O5G	0.189(14)	0.189(14)	0.188(14)	0.016(3)	0.006(3)	0.072(6)
O9X	0.061(11)	0.108(16)	0.100(15)	0.020(13)	-0.004(10)	0.036(11)
O10X	0.116(8)	0.119(8)	0.117(8)	0.010(3)	0.004(3)	0.045(4)
O11X	0.121(9)	0.122(9)	0.122(9)	0.010(3)	0.006(3)	0.044(4)

Table S22. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å2) for compound **5**.

	x/a	y/b	z/c	U(eq)
H02A	0.4771	-0.2279	0.4053	0.039000
H3G1	0.6085	-0.0234	0.5691	0.074000
H3G2	0.6364	0.0904	0.5914	0.074000
H3G3	0.5750	0.0010	0.6256	0.074000
H3GA	-0.1037	-0.0812	0.4450	0.073000
H2FA	0.6260	0.2016	0.6993	0.061000
H3CA	0.7667	0.9727	0.6406	0.087000
H2DA	0.4889	1.4163	0.9759	0.068000
H3FA	0.5701	0.4082	0.7608	0.060000
H8FA	0.4933	0.3304	0.6497	0.035000

H7FA	0.6969	0.4811	0.6988	0.031000
H3C1	1.3930	1.3290	0.8881	0.072000
H3C2	1.4546	1.2794	0.8523	0.072000
H3C3	1.4481	1.3828	0.8389	0.072000
H4CA	1.3889	1.2463	0.7461	0.044000
H7CA	0.9925	1.2476	0.7193	0.039000
H2CB	0.8924	1.1522	0.7947	0.082000
H2EA	0.3305	-0.3885	0.4318	0.103000
H4FA	0.7546	0.5661	0.5798	0.043000
H6FA	0.7692	0.3503	0.6763	0.036000
H6GA	0.2121	0.0368	0.4299	0.038000
H5CA	1.0488	1.2374	0.5266	0.088000
H2GB	0.1473	0.1637	0.4375	0.073000
H5FA	0.6681	0.2861	0.5749	0.038000
H2BA	-0.3462	0.5684	1.0133	0.091000
H1D1	0.1864	1.4495	1.2968	0.087000
H1D2	0.1111	1.3397	1.2756	0.087000
H1D3	0.2197	1.3563	1.2990	0.087000
H1A1	1.6447	1.1801	0.0436	0.095000
H1A2	1.6714	1.1071	0.0789	0.095000
H1A3	1.6469	1.0766	0.0183	0.095000
H5FB	0.5847	0.6470	0.6557	0.082000
H10B	1.0620	1.2607	0.6215	0.048000
H10C	1.1356	1.1969	0.5976	0.048000
H3AA	1.1386	0.7287	0.2096	0.082000
H6EA	0.6295	-0.3763	0.4650	0.044000
H3BB	-0.3584	0.3865	0.8471	0.088000

H10A	-0.2165	0.4179	0.9015	0.045000
H3F1	1.1048	0.7213	0.5416	0.083000
H3F2	1.1469	0.6588	0.5768	0.083000
H3F3	1.1265	0.6277	0.5160	0.083000
H6AA	1.2628	0.8868	0.1881	0.050000
H6BA	-0.2838	0.4503	1.0533	0.055000
H7GA	0.0386	-0.0443	0.3906	0.042000
H9FA	0.4646	0.4850	0.6214	0.052000
H9FB	0.4758	0.4908	0.6883	0.052000
H4BA	0.0834	0.4055	1.0068	0.062000
H4GA	0.3093	-0.0922	0.4645	0.046000
H3EB	0.5661	-0.4420	0.5462	0.118000
H5EA	0.4738	-0.4299	0.4010	0.048000
H5GA	0.1342	0.0088	0.5438	0.037000
H8BA	-0.4268	0.3002	0.9468	0.040000
H3FB	0.9164	0.6923	0.5563	0.048000
H6CA	0.9756	1.0319	0.7526	0.044000
H11A	-0.1974	0.5694	0.9687	0.047000
H1CA	1.2264	1.1669	0.6964	0.045000
H8DA	0.3059	1.4563	1.2231	0.049000
H8DB	0.1887	1.4384	1.1978	0.049000
H2EB	0.8665	-0.1788	0.3348	0.064000
H4EB	0.7534	-0.1818	0.4112	0.050000
H8GA	-0.0236	-0.2143	0.4485	0.055000
H4AA	1.2756	1.0733	0.0705	0.080000
H7AA	1.1610	0.9857	0.2007	0.078000
H3GB	0.4905	-0.0356	0.4863	0.049000

H3GC	0.4277	-0.1293	0.5252	0.049000
H7DA	0.2606	1.2589	1.2086	0.058000
H7DB	0.1458	1.2437	1.1810	0.058000
H6DA	0.1342	1.2378	1.0767	0.053000
H5BA	-0.0979	0.3577	0.9820	0.051000
H9CA	0.9508	1.0205	0.5979	0.057000
H8CA	0.8535	1.1491	0.6375	0.062000
H2B1	0.2200	0.5095	1.0818	0.089000
H2B2	0.2198	0.6182	1.0983	0.089000
H2B3	0.1751	0.5302	1.1359	0.089000
H3DA	0.5105	1.4421	1.0734	0.062000
H8EA	0.7110	-0.2538	0.5700	0.056000
H8EB	0.7628	-0.2103	0.5125	0.056000
H7EA	0.5425	-0.2506	0.5391	0.044000
H3AB	1.4558	1.1779	0.0531	0.084000
H1BA	-0.2531	0.1522	0.8792	0.106000
H2E1	0.7466	-0.2660	0.1984	0.108000
H2E2	0.8419	-0.1730	0.2228	0.108000
H2E3	0.8315	-0.2849	0.2308	0.108000
H4AB	1.0892	0.8731	0.2634	0.102000
H12A	-0.3913	0.1448	0.9328	0.054000
H12B	-0.3971	0.1952	0.8752	0.054000
H9GA	0.0885	-0.1935	0.3603	0.131000
H9GB	0.1965	-0.1265	0.3984	0.131000
H5AA	1.1681	0.7979	0.0820	0.066000
H8AA	0.9899	0.8281	0.1286	0.076000
H2DB	0.4273	1.3873	1.1599	0.059000

H9AA	0.9333	0.9736	0.1629	0.110000
H9AB	1.0344	1.0563	0.1334	0.110000
H5GB	0.1613	-0.3074	0.3911	0.283000

Table S23. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å2) for compound **6**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)
W1	0.59060(3)	0.68202(2)	0.57493(2)	0.01472(10)
W2	0.58038(3)	0.58185(2)	0.70104(2)	0.01559(11)
W3	0.79069(3)	0.78759(2)	0.60899(2)	0.01528(10)
W4	0.57237(3)	0.78010(2)	0.72923(2)	0.01410(10)
W5	0.78012(3)	0.58810(2)	0.59260(2)	0.01617(11)
W6	0.95020(3)	0.67333(2)	0.90597(2)	0.01547(11)
W7	0.96190(3)	0.78364(2)	0.76698(3)	0.01652(11)
W8	0.74305(3)	0.77624(2)	0.88583(2)	0.01396(10)
W9	0.76920(4)	0.57688(2)	0.87298(2)	0.01717(11)
W10	0.56284(3)	0.68017(2)	0.85634(3)	0.01663(11)
W11	0.96840(4)	0.58447(2)	0.76485(3)	0.01839(11)
W12	0.97808(3)	0.69479(2)	0.62631(3)	0.01872(11)
Si1	0.7709(2)	0.68225(11)	0.74045(16)	0.01617(11)
O5	0.8370(6)	0.7204(3)	0.9218(4)	0.0155(15)
O6	0.9910(6)	0.7264(3)	0.8375(4)	0.0177(16)
O7	0.5461(6)	0.7275(3)	0.6518(4)	0.0184(16)
O9	0.6918(5)	0.7170(3)	0.7867(4)	0.0101(14)

C14	0.7487(9)	0.4320(5)	0.7378(7)	0.023(2)
O10	0.6853(5)	0.8014(3)	0.6755(4)	0.0135(14)
O11	0.6671(6)	0.6301(3)	0.8909(4)	0.0203(16)
O12	0.5361(6)	0.6335(3)	0.7697(4)	0.0183(16)
O13	0.5199(6)	0.6237(3)	0.6163(4)	0.0194(16)
O14	0.8456(6)	0.7982(3)	0.8233(4)	0.0170(15)
O15	0.8760(6)	0.6452(3)	0.5834(4)	0.0192(16)
O16	0.8694(6)	0.6157(3)	0.9406(4)	0.0179(16)
O17	0.0086(6)	0.6428(3)	0.7056(5)	0.0216(17)
O18	0.7398(7)	0.5272(3)	0.9336(5)	0.0283(19)
O19	0.8857(6)	0.5444(3)	0.8297(4)	0.0211(16)
O20	0.6316(6)	0.7339(3)	0.9197(4)	0.0171(15)
O21	0.6994(6)	0.7327(3)	0.5659(4)	0.0213(17)
O22	0.6693(6)	0.5497(3)	0.6306(4)	0.0196(16)
O23	0.4978(6)	0.7368(3)	0.7950(4)	0.0188(16)
O24	0.6770(6)	0.6300(3)	0.5297(4)	0.0207(17)
O25	0.9051(6)	0.7514(3)	0.5704(4)	0.0203(16)
O10Z	0.9288(11)	0.4189(6)	0.9190(8)	0.072(4)
O26	0.8473(6)	0.7220(3)	0.6997(4)	0.0158(15)
N13	0.6055(8)	0.4327(4)	0.6381(6)	0.028(2)
O27	0.8399(6)	0.6434(3)	0.7998(4)	0.0122(14)
O28	0.7707(7)	0.8380(3)	0.5439(5)	0.0243(18)
O29	0.0276(6)	0.6216(3)	0.8557(4)	0.0209(16)
O30	0.8902(7)	0.8214(3)	0.6821(4)	0.0202(17)
O31	0.7609(7)	0.8202(3)	0.9606(4)	0.0209(17)
O32	0.0406(6)	0.7480(3)	0.6962(5)	0.0223(17)
O33	0.7045(6)	0.6464(3)	0.6754(4)	0.0135(14)

O34	0.6816(6)	0.5609(3)	0.7825(4)	0.0199(16)
O35	0.6394(6)	0.8137(3)	0.8204(4)	0.0176(16)
O36	0.5043(7)	0.6957(3)	0.4980(5)	0.0272(19)
O37	0.8698(6)	0.5683(3)	0.6801(5)	0.0227(17)
O38	0.8152(8)	0.5440(4)	0.5256(5)	0.033(2)
O11A	0.9188(7)	0.4352(4)	0.6975(6)	0.041(2)
O39	0.0329(7)	0.6829(3)	0.9871(5)	0.030(2)
N15	0.7584(10)	0.4329(4)	0.8174(6)	0.032(3)
O9Z	0.5849(8)	0.5586(5)	0.4213(7)	0.051(3)
N4	0.7528(9)	0.7850(5)	0.3354(6)	0.036(3)
C12	0.6743(9)	0.4334(5)	0.5870(7)	0.026(3)
O40	0.0771(7)	0.6836(4)	0.5711(5)	0.033(2)
O1	0.4800(7)	0.8265(3)	0.7027(5)	0.0239(18)
O2	0.4897(7)	0.5330(3)	0.7034(5)	0.030(2)
O3	0.0470(7)	0.8314(4)	0.8010(5)	0.032(2)
O4	0.4662(7)	0.6632(4)	0.9103(5)	0.030(2)
O5A	0.0655(7)	0.5399(3)	0.7543(5)	0.0292(19)
N3	0.7797(8)	0.7482(5)	0.2111(6)	0.027(2)
N12	0.7785(9)	0.4342(4)	0.6089(7)	0.030(2)
N14	0.5915(9)	0.4348(4)	0.7765(6)	0.028(2)
N2	0.8024(9)	0.8145(5)	0.1212(6)	0.032(3)
C13	0.6456(10)	0.4328(4)	0.7138(8)	0.027(3)
C15	0.8257(9)	0.4339(5)	0.6841(7)	0.026(3)
O1A	0.7849(9)	0.9038(4)	0.1415(6)	0.048(3)
C3	0.7740(10)	0.8425(6)	0.2437(7)	0.032(3)
N5	0.7596(9)	0.8696(5)	0.3099(6)	0.036(3)
N1	0.8099(11)	0.7274(5)	0.0884(7)	0.042(3)

N11	0.6426(10)	0.4353(5)	0.5138(7)	0.039(3)
C11	0.6613(11)	0.4343(5)	0.8372(7)	0.031(3)
C4	0.7982(9)	0.7627(5)	0.1392(6)	0.025(3)
C5	0.7873(10)	0.8588(6)	0.1680(8)	0.031(3)
C2	0.7689(10)	0.7893(6)	0.2603(7)	0.032(3)
O8Z	0.2579(10)	0.8519(5)	0.7576(7)	0.055(3)
O7Z	0.1143(10)	0.4319(5)	0.7895(10)	0.071(4)
O6Z	0.0672(10)	0.4828(6)	0.6007(7)	0.062(3)
O5Z	0.7274(9)	0.5144(5)	0.3363(8)	0.057(3)
O4Z	0.1018(12)	0.5721(5)	0.5118(8)	0.067(4)
C1	0.7485(11)	0.8350(7)	0.3631(8)	0.043(4)
O3Z	0.3882(10)	0.4384(6)	0.7934(9)	0.071(4)
O2Z	0.2725(12)	0.8080(6)	0.9104(8)	0.072(4)
O1Z	0.7839(12)	0.6166(7)	0.0863(9)	0.080(4)
O11Z	0.4687(13)	0.8479(8)	0.9113(10)	0.101(6)
O12Z	0.7905(14)	0.9697(8)	0.3668(10)	0.097(5)
O13Z	0.0965(18)	0.5124(10)	0.9431(13)	0.135(8)
O14Z	0.446(2)	0.5545(11)	0.0002(16)	0.155(9)
O15Z	0.565(2)	0.6368(11)	0.0742(16)	0.156(9)

Table 24. Bond lengths (Å) for compound **6**.

W1-O36	1.697(8)	W1-O7	1.900(7)
W1-O13	1.903(8)	W1-O21	1.910(8)
W1-O24	1.935(8)	W1-O33	2.354(7)
W2-O2	1.695(9)	W2-O12	1.896(7)
W2-O34	1.910(8)	W2-O13	1.920(8)
W2-O22	1.946(8)	W2-O33	2.350(7)

W3-O28	1.704(7)	W3-O21	1.914(8)
W3-O10	1.914(7)	W3-O25	1.915(8)
W3-O30	1.918(8)	W3-O26	2.351(7)
W4-O1	1.695(7)	W4-O10	1.893(7)
W4-O7	1.898(7)	W4-O23	1.913(8)
W4-O35	1.933(8)	W4-O9	2.358(7)
W5-O38	1.709(8)	W5-O37	1.894(8)
W5-O22	1.900(8)	W5-O15	1.906(8)
W5-O24	1.947(8)	W5-O33	2.343(7)
W6-O39	1.708(8)	W6-O6	1.901(8)
W6-O29	1.906(8)	W6-O16	1.913(8)
W6-O5	1.918(8)	W6-O27	2.351(7)
W7-O3	1.689(8)	W7-O32	1.906(8)
W7-O6	1.906(7)	W7-O14	1.917(8)
W7-O30	1.920(8)	W7-O26	2.366(7)
W8-O31	1.711(7)	W8-O14	1.887(8)
W8-O5	1.914(7)	W8-O35	1.917(7)
W8-O20	1.929(8)	W8-O9	2.331(7)
W9-O18	1.704(8)	W9-O34	1.898(8)
W9-O11	1.921(8)	W9-O16	1.926(7)
W9-O19	1.933(8)	W9-O27	2.344(7)
W10-O4	1.697(8)	W10-O11	1.892(8)
W10-O20	1.906(7)	W10-O12	1.921(7)
W10-O23	1.921(8)	W10-O9	2.353(7)
W11-O5A	1.700(8)	W11-O17	1.896(8)
W11-O37	1.901(8)	W11-O19	1.922(8)
W11-O29	1.936(8)	W11-O27	2.347(7)

W12-O40	1.705(9)	W12-O15	1.908(8)
W12-O25	1.914(8)	W12-O17	1.916(8)
W12-O32	1.930(8)	W12-O26	2.330(8)
Si1-O26	1.618(8)	Si1-O9	1.621(7)
Si1-O27	1.623(7)	Si1-O33	1.626(7)
C14-C13	1.354(17)	C14-N15	1.394(16)
C14-C15	1.440(17)	N13-C12	1.328(16)
N13-C13	1.377(17)	O11A-C15	1.201(16)
N15-C11	1.336(19)	N4-C1	1.34(2)
N4-C2	1.362(17)	C12-N11	1.311(17)
C12-N12	1.361(16)	N3-C4	1.360(16)
N3-C21	.359(18)	N12-C15	1.398(16)
N14-C11	1.324(17)	N14-C13	1.366(17)
N2-C4	1.335(17)	N2-C5	1.404(17)
O1A-C5	1.218(17)	C3-C2	1.36(2)
C3-N5	1.376(16)	C3-C5	1.420(18)
N5-C1	1.29(2)	N1-C4	1.276(17)

Table S25. Bond angles (°) for compound **6**.

O36-W1-O7	103.0(4)	O36-W1-O13	99.1(4)
O7-W1-O13	89.7(3)	O36-W1-O21	103.2(4)
O7-W1-O21	86.6(3)	O13-W1-O21	157.7(3)
O36-W1-O24	99.6(4)	O7-W1-O24	157.4(3)
O13-W1-O24	87.8(3)	O21-W1-O24	87.2(3)
O36-W1-O33	169.4(3)	O7-W1-O33	84.5(3)
O13-W1-O33	73.2(3)	O21-W1-O33	84.5(3)
O24-W1-O33	73.3(3)	O2-W2-O12	102.8(4)

O2-W2-O34	101.8(4)	O12-W2-O34	86.4(3)
O2-W2-O13	100.7(4)	O12-W2-O13	89.9(3)
O34-W2-O13	157.5(3)	O2-W2-O22	99.9(4)
O12-W2-O22	157.3(3)	O34-W2-O22	87.8(3)
O13-W2-O22	87.2(3)	O2-W2-O33	170.2(4)
O12-W2-O33	84.8(3)	O34-W2-O33	84.6(3)
O13-W2-O33	73.0(3)	O22-W2-O33	72.7(3)
O28-W3-O21	102.7(4)	O28-W3-O10	102.1(4)
O21-W3-O10	85.6(3)	O28-W3-O25	100.4(4)
O21-W3-O25	89.2(3)	O10-W3-O25	157.5(3)
O28-W3-O30	99.8(4)	O21-W3-O30	157.5(3)
O10-W3-O30	88.9(3)	O25-W3-O30	87.6(3)
O28-W3-O26	170.6(3)	O21-W3-O26	84.5(3)
O10-W3-O26	84.4(3)	O25-W3-O26	73.4(3)
O30-W3-O26	73.2(3)	O1-W4-O10	103.0(4)
O1-W4-O7	102.0(4)	O10-W4-O7	85.8(3)
O1-W4-O23	99.8(4)	O10-W4-O23	157.1(3)
O7-W4-O23	88.8(3)	O1-W4-O35	100.0(3)
O10-W4-O35	89.4(3)	O7-W4-O35	158.0(3)
O23-W4-O35	87.4(3)	O1-W4-O9	170.5(3)
O10-W4-O9	84.2(3)	O7-W4-O9	84.6(3)
O23-W4-O9	73.2(3)	O35-W4-O9	73.6(3)
O38-W5-O37	102.0(4)	O38-W5-O22	100.3(4)
O37-W5-O22	90.1(3)	O38-W5-O15	101.8(4)
O37-W5-O15	85.3(3)	O22-W5-O15	157.9(3)
O38-W5-O24	99.8(4)	O37-W5-O24	158.0(3)
O22-W5-O24	88.6(3)	O15-W5-O24	87.7(3)

O38-W5-O33	170.7(4)	O37-W5-O33	85.2(3)
O22-W5-O33	73.7(3)	O15-W5-O33	84.4(3)
O24-W5-O33	73.4(3)	O39-W6-O6	103.9(4)
O39-W6-O29	99.8(4)	O6-W6-O29	89.2(3)
O39-W6-O16	98.9(4)	O6-W6-O16	157.2(3)
O29-W6-O16	88.0(3)	O39-W6-O5	102.3(4)
O6-W6-O5	85.9(3)	O29-W6-O5	157.9(3)
O16-W6-O5	88.2(3)	O39-W6-O27	169.5(3)
O6-W6-O27	84.5(3)	O29-W6-O27	73.7(3)
O16-W6-O27	73.0(3)	O5-W6-O27	84.4(3)
O3-W7-O32	101.0(4)	O3-W7-O6	102.8(4)
O32-W7-O6	89.5(3)	O3-W7-O14	101.4(4)
O32-W7-O14	157.6(3)	O6-W7-O14	85.4(3)
O3-W7-O30	99.9(4)	O32-W7-O30	88.2(4)
O6-W7-O30	157.2(3)	O14-W7-O30	88.1(3)
O3-W7-O26	170.8(4)	O32-W7-O26	73.6(3)
O6-W7-O26	84.7(3)	O14-W7-O26	84.2(3)
O30-W7-O26	72.8(3)	O31-W8-O14	102.3(4)
O31-W8-O5	100.6(3)	O14-W8-O5	86.9(3)
O31-W8-O35	100.3(3)	O14-W8-O35	89.7(3)
O5-W8-O35	159.1(3)	O31-W8-O20	99.3(4)
O14-W8-O20	158.4(3)	O5-W8-O20	88.0(3)
O35-W8-O20	87.5(3)	O31-W8-O9	171.2(3)
O14-W8-O9	84.9(3)	O5-W8-O9	84.6(3)
O35-W8-O9	74.6(3)	O20-W8-O9	73.7(3)
O18-W9-O34	102.7(4)	O18-W9-O11	101.6(4)
O34-W9-O11	85.6(3)	O18-W9-O16	99.2(4)

O34-W9-O16	158.1(3)	O11-W9-O16	88.8(3)
O18-W9-O19	99.9(4)	O34-W9-O19	90.1(3)
O11-W9-O19	158.5(3)	O16-W9-O19	87.4(3)
O18-W9-O27	169.8(4)	O34-W9-O27	85.5(3)
O11-W9-O27	84.9(3)	O16-W9-O27	73.0(3)
O19-W9-O27	73.7(3)	O4-W10-O11	101.2(4)
O4-W10-O20	100.0(4)	O11-W10-O20	90.3(3)
O4-W10-O12	102.1(4)	O11-W10-O12	85.3(3)
O20-W10-O12	157.9(3)	O4-W10-O23	101.2(4)
O11-W10-O23	157.5(3)	O20-W10-O23	87.7(3)
O12-W10-O23	88.2(3)	O4-W10-O9	171.4(4)
O11-W10-O9	84.8(3)	O20-W10-O9	73.6(3)
O12-W10-O9	84.5(3)	O23-W10-O9	73.2(3)
O5A-W11-O17	101.4(4)	O5A-W11-O37	102.5(4)
O17-W11-O37	86.1(3)	O5A-W11-O19	100.6(4)
O17-W11-O19	158.0(3)	O37-W11-O19	89.2(3)
O5A-W11-O29	99.9(4)	O17-W11-O29	88.7(3)
O37-W11-O29	157.6(3)	O19-W11-O29	87.5(3)
O5A-W11-O27	171.1(4)	O17-W11-O27	84.3(3)
O37-W11-O27	84.5(3)	O19-W11-O27	73.8(3)
O29-W11-O27	73.3(3)	O40-W12-O15	101.3(4)
O40-W12-O25	100.8(4)	O15-W12-O25	89.6(3)
O40-W12-O17	101.1(4)	O15-W12-O17	86.0(3)
O25-W12-O17	158.1(3)	O40-W12-O32	100.7(4)
O15-W12-O32	157.9(3)	O25-W12-O32	88.2(3)
O17-W12-O32	87.9(3)	O40-W12-O26	172.4(4)
O15-W12-O26	84.2(3)	O25-W12-O26	73.9(3)

O17-W12-O26	84.3(3)	O32-W12-O26	74.0(3)
O26-Si1-O9	109.6(4)	O26-Si1-O27	109.4(4)
O9-Si1-O27	109.3(4)	O26-Si1-O33	109.2(4)
O9-Si1-O33	109.5(4)	O27-Si1-O33	109.7(4)
W8-O5-W6	150.0(4)	W6-O6-W7	152.5(4)
W4-O7-W1	151.6(5)	Si1-O9-W8	124.8(4)
Si1-O9-W10	124.5(4)	W8-O9-W10	91.2(2)
Si1-O9-W4	124.1(4)	W8-O9-W4	91.1(2)
W10-O9-W4	91.1(2)	C13-C14-N15	107.3(11)
C13-C14-C15	121.2(11)	N15-C14-C15	131.3(11)
W4-O10-W3	152.4(4)	W10-O11-W9	152.0(4)
W2-O12-W10	151.3(5)	W1-O13-W2	122.8(4)
W8-O14-W7	151.5(4)	W5-O15-W12	151.7(4)
W6-O16-W9	122.4(4)	W11-O17-W12	150.9(5)
W11-O19-W9	121.1(4)	W10-O20-W8	121.5(4)
W1-O21-W3	150.6(5)	W5-O22-W2	122.0(4)
W4-O23-W10	122.6(4)	W1-O24-W5	121.2(4)
W12-O25-W3	121.6(4)	Si1-O26-W12	125.1(4)
Si1-O26-W3	124.6(4)	W12-O26-W3	91.1(3)
Si1-O26-W7	123.9(4)	W12-O26-W7	90.9(3)
W3-O26-W7	91.2(3)	C12-N13-C13	116.3(11)
Si1-O27-W9	124.0(4)	Si1-O27-W11	124.3(4)
W9-O27-W11	91.4(2)	Si1-O27-W6	124.6(4)
W9-O27-W6	91.6(2)	W11-O27-W6	91.2(2)
W6-O29-W11	121.8(4)	W3-O30-W7	122.7(4)
W7-O32-W12	121.5(4)	Si1-O33-W5	123.8(4)
Si1-O33-W2	124.3(4)	W5-O33-W2	91.6(2)

Si1-O33-W1	124.3(4)	W5-O33-W1	92.1(2)
W2-O33-W1	91.0(2)	W9-O34-W2	150.9(5)
W8-O35-W4	120.8(4)	W5-O37-W11	152.3(5)
C11-N15-C14	105.8(11)	C1-N4-C2	107.2(13)
N11-C12-N13	120.2(12)	N11-C12-N12	118.5(12)
N13-C12-N12	121.2(12)	C4-N3-C2	115.4(12)
C12-N12-C15	126.2(11)	C11-N14-C13	106.8(11)
C4-N2-C5	127.9(11)	C14-C13-N14	108.5(12)
C14-C13-N13	124.1(12)	N14-C13-N13	127.4(11)
O11A-C15-N12	121.0(12)	O11A-C15-C14	128.1(12)
N12-C15-C14	110.9(10)	C2-C3-N5	106.6(12)
C2-C3-C5	119.5(13)	N5-C3-C5	133.8(14)
C1-N5-C3	108.5(13)	N14-C11-N15	111.6(12)
N1-C4-N2	119.7(12)	N1-C4-N3	120.7(13)
N2-C4-N3	119.6(11)	O1A-C5-N2	120.3(12)
O1A-C5-C3	128.5(13)	N2-C5-C3	111.2(12)
N3-C2-N4	126.4(14)	N3-C2-C3	126.2(12)
N4-C2-C3	107.4(13)	N5-C1-N4	110.3(12)

Table 26. Bond angles (°) for compound **6**.

O36-W1-O7	103.0(4)	O36-W1-O13	99.1(4)
O7-W1-O13	89.7(3)	O36-W1-O21	103.2(4)
O7-W1-O21	86.6(3)	O13-W1-O21	157.7(3)
O36-W1-O24	99.6(4)	O7-W1-O24	157.4(3)

O13-W1-O24	87.8(3)	O21-W1-O24	87.2(3)
O36-W1-O33	169.4(3)	O7-W1-O33	84.5(3)
O13-W1-O33	73.2(3)	O21-W1-O33	84.5(3)
O24-W1-O33	73.3(3)	O2-W2-O12	102.8(4)
O2-W2-O34	101.8(4)	O12-W2-O34	86.4(3)
O2-W2-O13	100.7(4)	O12-W2-O13	89.9(3)
O34-W2-O13	157.5(3)	O2-W2-O22	99.9(4)
O12-W2-O22	157.3(3)	O34-W2-O22	87.8(3)
O13-W2-O22	87.2(3)	O2-W2-O33	170.2(4)
O12-W2-O33	84.8(3)	O34-W2-O33	84.6(3)
O13-W2-O33	73.0(3)	O22-W2-O33	72.7(3)
O28-W3-O21	102.7(4)	O28-W3-O10	102.1(4)
O21-W3-O10	85.6(3)	O28-W3-O25	100.4(4)
O21-W3-O25	89.2(3)	O10-W3-O25	157.5(3)
O28-W3-O30	99.8(4)	O21-W3-O30	157.5(3)
O10-W3-O30	88.9(3)	O25-W3-O30	87.6(3)
O28-W3-O26	170.6(3)	O21-W3-O26	84.5(3)
O10-W3-O26	84.4(3)	O25-W3-O26	73.4(3)
O30-W3-O26	73.2(3)	O1-W4-O10	103.0(4)
O1-W4-O7	102.0(4)	O10-W4-O7	85.8(3)
O1-W4-O23	99.8(4)	O10-W4-O23	157.1(3)
O7-W4-O23	88.8(3)	O1-W4-O35	100.0(3)
O10-W4-O35	89.4(3)	O7-W4-O35	158.0(3)
O23-W4-O35	87.4(3)	O1-W4-O9	170.5(3)
O10-W4-O9	84.2(3)	O7-W4-O9	84.6(3)
O23-W4-O9	73.2(3)	O35-W4-O9	73.6(3)
O38-W5-O37	102.0(4)	O38-W5-O22	100.3(4)

O37-W5-O22	90.1(3)	O38-W5-O15	101.8(4)
O37-W5-O15	85.3(3)	O22-W5-O15	157.9(3)
O38-W5-O24	99.8(4)	O37-W5-O24	158.0(3)
O22-W5-O24	88.6(3)	O15-W5-O24	87.7(3)
O38-W5-O33	170.7(4)	O37-W5-O33	85.2(3)
O22-W5-O33	73.7(3)	O15-W5-O33	84.4(3)
O24-W5-O33	73.4(3)	O39-W6-O6	103.9(4)
O39-W6-O29	99.8(4)	O6-W6-O29	89.2(3)
O39-W6-O16	98.9(4)	O6-W6-O16	157.2(3)
O29-W6-O16	88.0(3)	O39-W6-O5	102.3(4)
O6-W6-O5	85.9(3)	O29-W6-O5	157.9(3)
O16-W6-O5	88.2(3)	O39-W6-O27	169.5(3)
O6-W6-O27	84.5(3)	O29-W6-O27	73.7(3)
O16-W6-O27	73.0(3)	O5-W6-O27	84.4(3)
O3-W7-O32	101.0(4)	O3-W7-O6	102.8(4)
O32-W7-O6	89.5(3)	O3-W7-O14	101.4(4)
O32-W7-O14	157.6(3)	O6-W7-O14	85.4(3)
O3-W7-O30	99.9(4)	O32-W7-O30	88.2(4)
O6-W7-O30	157.2(3)	O14-W7-O30	88.1(3)
O3-W7-O26	170.8(4)	O32-W7-O26	73.6(3)
O6-W7-O26	84.7(3)	O14-W7-O26	84.2(3)
O30-W7-O26	72.8(3)	O31-W8-O14	102.3(4)
O31-W8-O5	100.6(3)	O14-W8-O5	86.9(3)
O31-W8-O35	100.3(3)	O14-W8-O35	89.7(3)
O5-W8-O35	159.1(3)	O31-W8-O20	99.3(4)
O14-W8-O20	158.4(3)	O5-W8-O20	88.0(3)
O35-W8-O20	87.5(3)	O31-W8-O9	171.2(3)

O14-W8-O9	84.9(3)	O5-W8-O9	84.6(3)
O35-W8-O9	74.6(3)	O20-W8-O9	73.7(3)
O18-W9-O34	102.7(4)	O18-W9-O11	101.6(4)
O34-W9-O11	85.6(3)	O18-W9-O16	99.2(4)
O34-W9-O16	158.1(3)	O11-W9-O16	88.8(3)
O18-W9-O19	99.9(4)	O34-W9-O19	90.1(3)
O11-W9-O19	158.5(3)	O16-W9-O19	87.4(3)
O18-W9-O27	169.8(4)	O34-W9-O27	85.5(3)
O11-W9-O27	84.9(3)	O16-W9-O27	73.0(3)
O19-W9-O27	73.7(3)	O4-W10-O11	101.2(4)
O4-W10-O20	100.0(4)	O11-W10-O20	90.3(3)
O4-W10-O12	102.1(4)	O11-W10-O12	85.3(3)
O20-W10-O12	157.9(3)	O4-W10-O23	101.2(4)
O11-W10-O23	157.5(3)	O20-W10-O23	87.7(3)
O12-W10-O23	88.2(3)	O4-W10-O9	171.4(4)
O11-W10-O9	84.8(3)	O20-W10-O9	73.6(3)
O12-W10-O9	84.5(3)	O23-W10-O9	73.2(3)
O5A-W11-O17	101.4(4)	O5A-W11-O37	102.5(4)
O17-W11-O37	86.1(3)	O5A-W11-O19	100.6(4)
O17-W11-O19	158.0(3)	O37-W11-O19	89.2(3)
O5A-W11-O29	99.9(4)	O17-W11-O29	88.7(3)
O37-W11-O29	157.6(3)	O19-W11-O29	87.5(3)
O5A-W11-O27	171.1(4)	O17-W11-O27	84.3(3)
O37-W11-O27	84.5(3)	O19-W11-O27	73.8(3)
O29-W11-O27	73.3(3)	O40-W12-O15	101.3(4)
O40-W12-O25	100.8(4)	O15-W12-O25	89.6(3)
O40-W12-O17	101.1(4)	O15-W12-O17	86.0(3)

O25-W12-O17	158.1(3)	O40-W12-O32	100.7(4)
O15-W12-O32	157.9(3)	O25-W12-O32	88.2(3)
O17-W12-O32	87.9(3)	O40-W12-O26	172.4(4)
O15-W12-O26	84.2(3)	O25-W12-O26	73.9(3)
O17-W12-O26	84.3(3)	O32-W12-O26	74.0(3)
O26-Si1-O9	109.6(4)	O26-Si1-O27	109.4(4)
O9-Si1-O27	109.3(4)	O26-Si1-O33	109.2(4)
O9-Si1-O33	109.5(4)	O27-Si1-O33	109.7(4)
W8-O5-W6	150.0(4)	W6-O6-W7	152.5(4)
W4-O7-W1	151.6(5)	Si1-O9-W8	124.8(4)
Si1-O9-W10	124.5(4)	W8-O9-W10	91.2(2)
Si1-O9-W4	124.1(4)	W8-O9-W4	91.1(2)
W10-O9-W4	91.1(2)	C13-C14-N15	107.3(11)
C13-C14-C15	1 21.2(11)	N15-C14-C15	1 31.3(11)
W4-O10-W3	152.4(4)	W10-O11-W9	152.0(4)
W2-O12-W10	151.3(5)	W1-O13-W2	122.8(4)
W8-O14-W7	151.5(4)	W5-O15-W12	151.7(4)
W6-O16-W9	122.4(4)	W11-O17-W12	150.9(5)
W11-O19-W9	121.1(4)	W10-O20-W8	121.5(4)
W1-O21-W3	150.6(5)	W5-O22-W2	122.0(4)
W4-O23-W10	122.6(4)	W1-O24-W5	121.2(4)
W12-O25-W3	121.6(4)	Si1-O26-W12	125.1(4)
Si1-O26-W3	124.6(4)	W12-O26-W3	91.1(3)
Si1-O26-W7	123.9(4)	W12-O26-W7	90.9(3)
W3-O26-W7	91.2(3)	C12-N13-C13	1 16.3(11)
Si1-O27-W9	124.0(4)	Si1-O27-W11	124.3(4)
W9-O27-W11	91.4(2)	Si1-O27-W6	124.6(4)

W9-O27-W6	91.6(2)	W11-O27-W6	91.2(2)		
W6-O29-W11	121.8(4)	W3-O30-W7	122.7(4)		
W7-O32-W12	121.5(4)	Si1-O33-W5	123.8(4)		
Si1-O33-W2	124.3(4)	W5-O33-W2	91.6(2)		
Si1-O33-W1	124.3(4)	W5-O33-W1	92.1(2)		
W2-O33-W1	91.0(2)	W9-O34-W2	150.9(5)		
W8-O35-W4	120.8(4)	W5-O37-W11	152.3(5)		
C11-N15-C14	105.8(11)	C1-N4-C2	107.2(13)		
N11-C12-N13	120.2(12)	N11-C12-N12	118.5(12)		
N13-C12-N12	121.2(12)	C4-N3-C2	115.4(12)		
C12-N12-C15	126.2(11)	C11-N14-C13	106.8(11)		
C4-N2-C5	127.9(11)	C14-C13-N14	108.5(12)		
C14-C13-N13	124.1(12)	N14-C13-N13	127.4(11)		
O11A-C15-N12	121.0(12)	O11A-C15-C14	128.1(12)		
N12-C15-C14	110.9(10)	C2-C3-N5	106.6(12)		
C2-C3-C5	119.5(13)	N5-C3-C5	133.8(14)		
C1-N5-C3	108.5(13)	N14-C11-N15	111.6(12)		
N1-C4-N2	119.7(12)	N1-C4-N3	120.7(13)		
N2-C4-N3	119.6(11)	O1A-C5-N2	120.3(12)		
O1A-C5-C3	128.5(13)	N2-C5-C3	111.2(12)		
N3-C2-N4	126.4(14)	N3-C2-C3	126.2(12)		
N4-C2-C3	107.4(13)	N5-C1-N4	110.3(12)		

Table 28. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å2) for compound **6**.

	x/a	y/b	z/c	U(eq)
H4A	0.7465	0.7558	1.3603	0.043000

H12A	0.8192	0.4351	0.5731	0.036000
H14A	0.5249	0.4360	0.7766	0.034000
H2A	0.8160	0.8216	1.0754	0.038000
H1A	0.8052	0.6949	1.1087	0.063000
H1B	0.7604	0.7313	1.0497	0.063000
H1C	0.8721	0.7312	1.0715	0.063000
H11A	0.6975	0.4355	0.4871	0.058000
H11B	0.6034	0.4067	0.5009	0.058000
H11C	0.6053	0.4648	0.5037	0.058000
H11Z	0.6447	0.4349	0.8875	0.037000
H1Z	0.7389	0.8435	1.4134	0.051000