

Supporting Information

Durable and fast-response photochromic and switchable luminescent polyviologen-polyoxometalate hybrid

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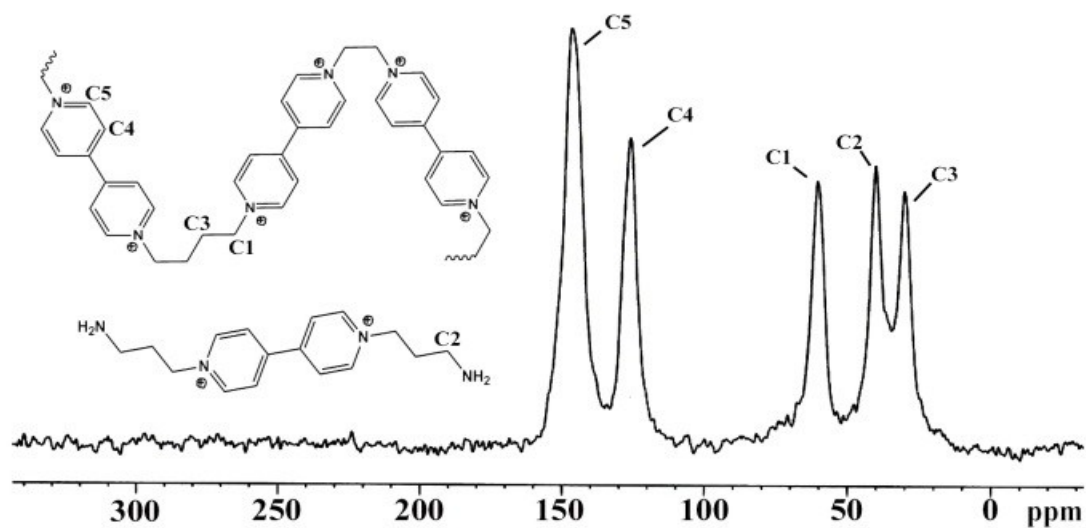


Figure S1. The solid state ^{13}C CP-MAS NMR of complex **1**.

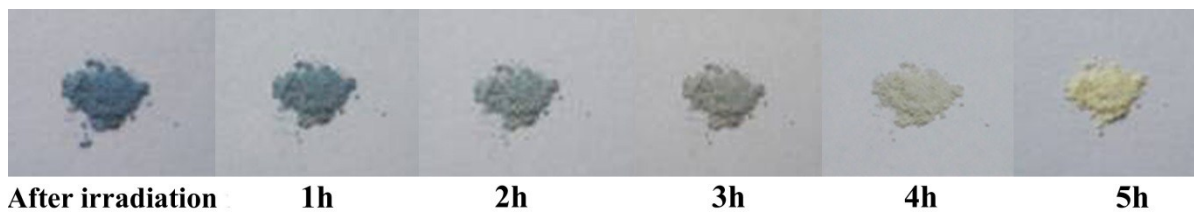


Figure S2. The color recovery process of complex **1** after 1, 2, 3, 4 and 5h in a dark box in air.

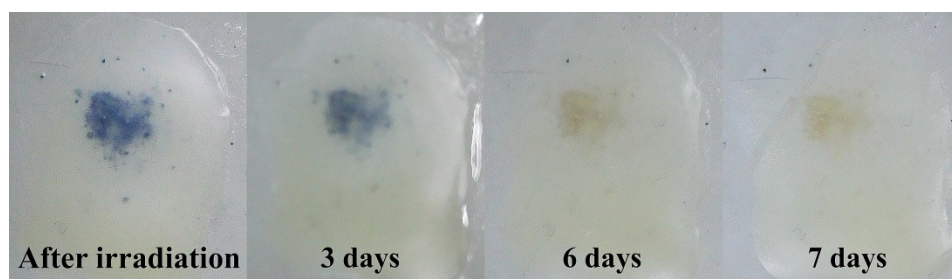


Figure S3. The color recovery process of complex **1** after 3, 6 and 7 days in a dark box in air. Complex **1** was wrapped by vaseline.

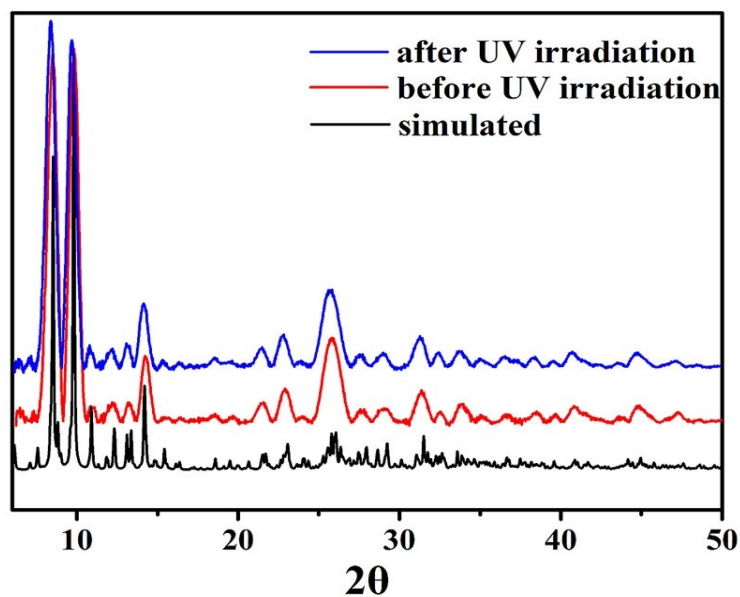


Figure S4. PXRD patterns of complex **1** before (red) and after (blue) UV irradiation with 300 W Hg lamp at room temperature in air for 30 min. The black line is simulated curve.

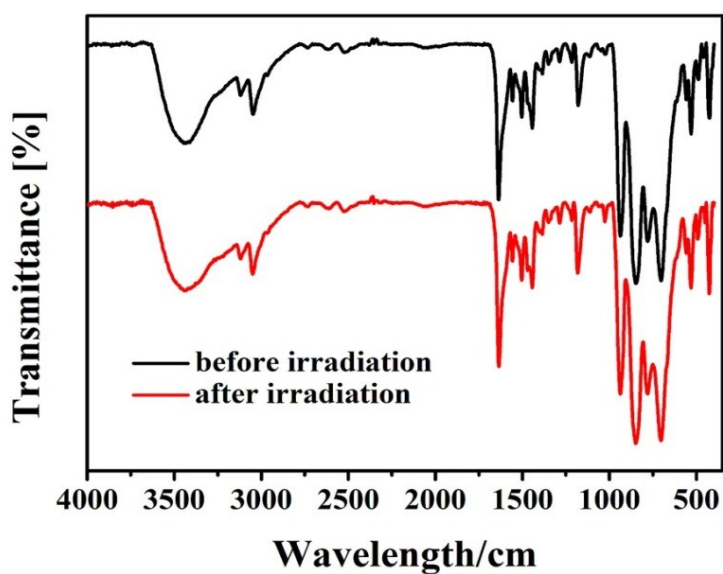


Figure S5. FTIR spectra of complex **1** before (black) and after (red) UV irradiation with 300W Hg lamp at room temperature in air for 5 min.

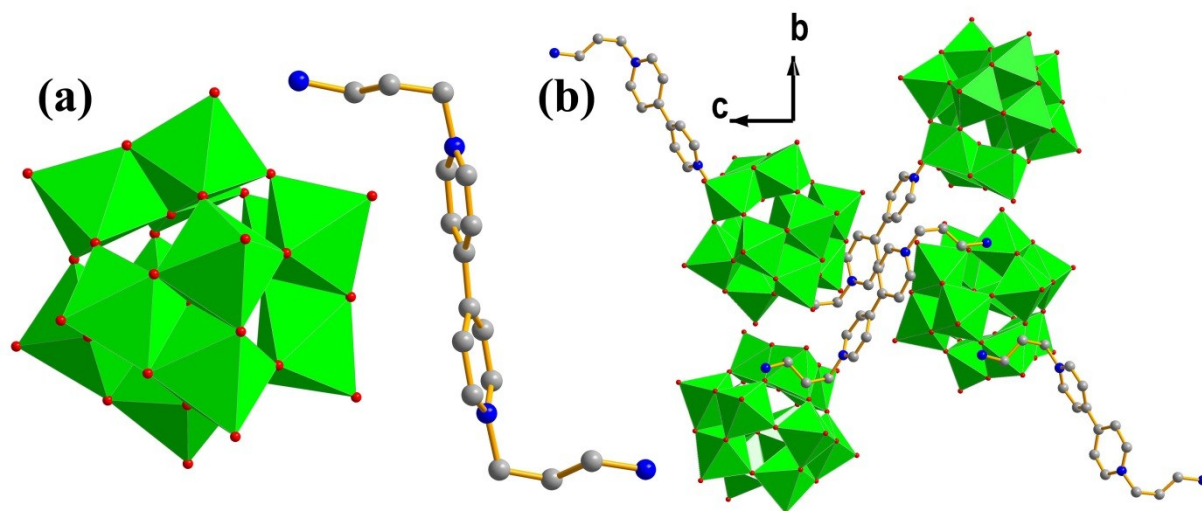


Figure S6 (a) A ball-and-stick and polyhedral combined view of complex **2**. (b) Packing diagram of complex **2** along *a* axis. Color code: C, gray; N, blue; O, brown. The isolated water molecules are omitted for clarity.

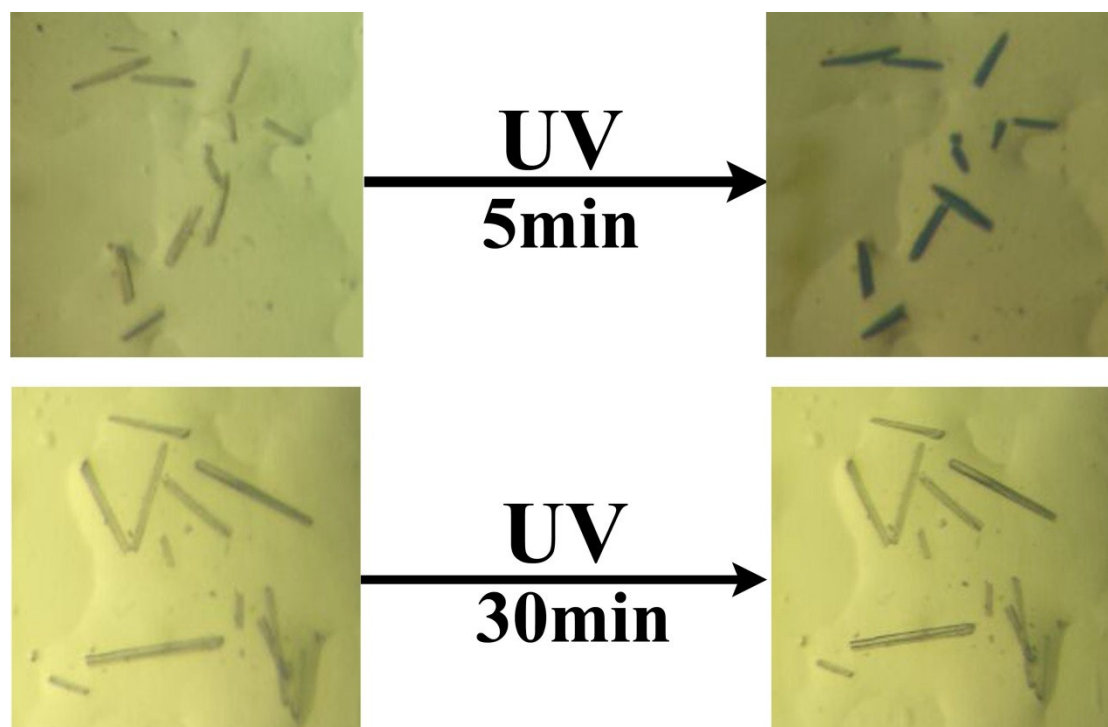


Figure S7 The photos of crystals **1** (top) and **2** (bottom) were recorded before irradiation (left) and after irradiation (right) by 300 W Hg lamp at room temperature in air.

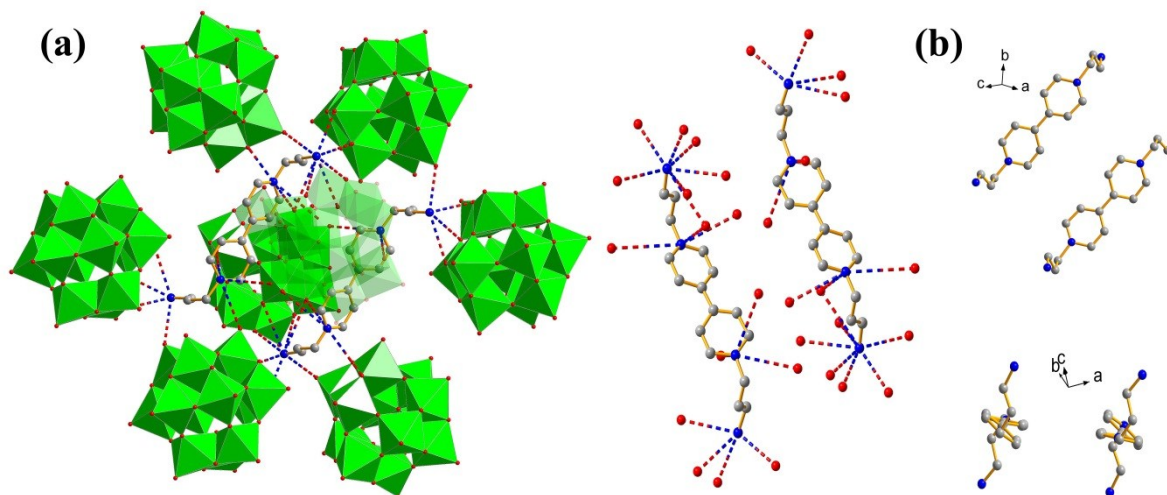


Figure S8 (a) A view of the weak interactions between AV^{2+} monomers and $Na_6[H_2W_{12}O_{40}] \cdot 20H_2O$. (b) The arrangement of AV^{2+} monomers. Color code: C, gray; N, blue; O, red. Isolated water molecules are omitted for clarity.

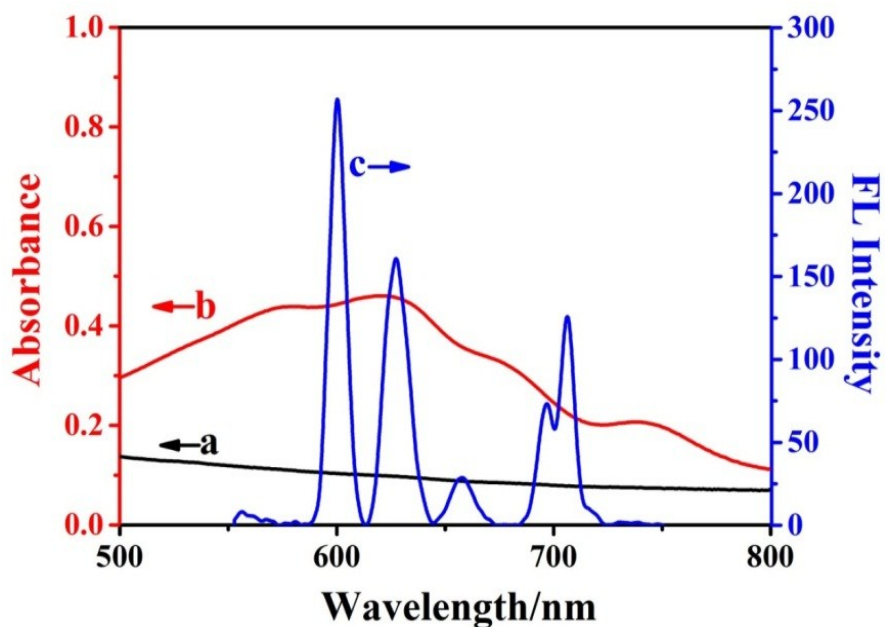


Figure S9. Absorption spectra of **1** before (a) and after exposure to UV irradiation (b) and fluorescent spectrum of complex **1** (c).

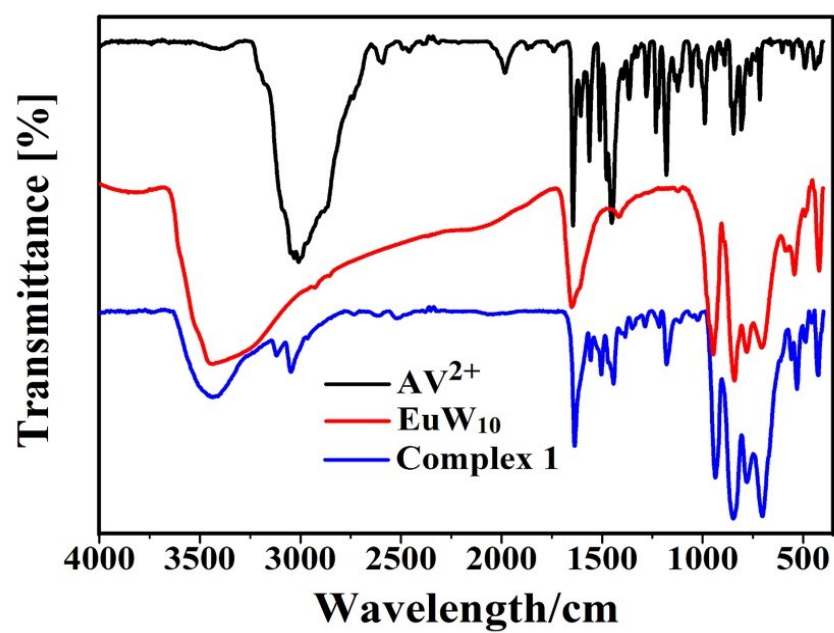


Figure S10 FTIR spectra of AV²⁺, EuW₁₀ and complex 1.

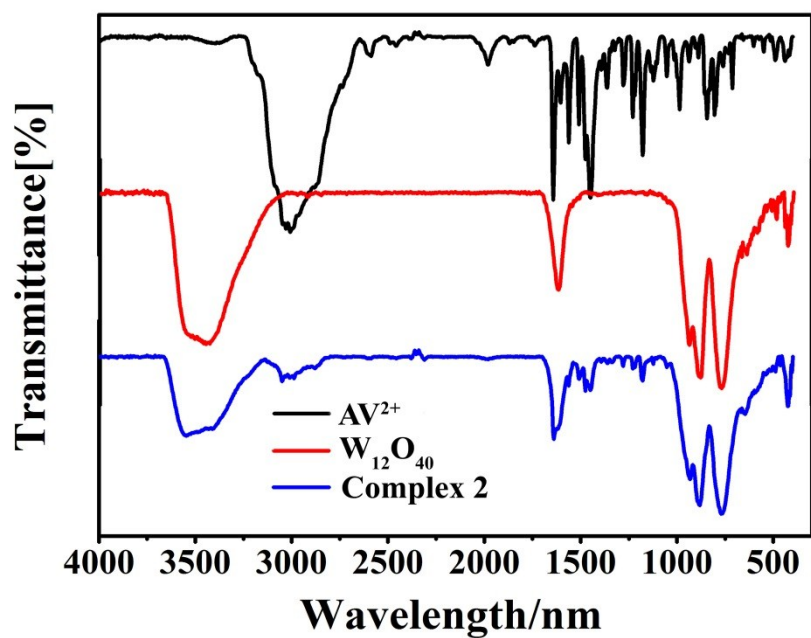


Figure S11 FTIR spectra of AV²⁺, Na₆[H₂W₁₂O₄₀]·20H₂O and complex 2.

Table S1. Crystal Data and Structure Refinements for **1** and **2**.

	1	2
Empirical formula	C ₃₆ H ₅₆ N ₇ O ₄₀ EuW ₁₀	C ₁₆ H ₃₆ N ₄ O ₄₅ W ₁₂
Formula weight	3217.22	3210.55
Temperature	293(2) K	293(2) K
Wavelength	0.71000 Å	0.71000 Å
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 21/ <i>n</i>	<i>P</i> 21/ <i>c</i>
<i>a</i> (Å)	14.4112(5)	12.0073(7)
<i>b</i> (Å)	19.9900(8)	20.1231(15)
<i>c</i> (Å)	20.8193(7)	23.5367(16)
α (deg)	90	90
β (deg)	96.156(4)	103.435(6)
γ (deg)	90	90
Volume	5963.0(4) Å ³	5531.4(6) Å ³
Z, Calculated density	4, 3.585 mg/m ³	4, 3.857 mg/m ³
Absorption coefficient	20.340 mm ⁻¹	24.941 mm ⁻¹
F(000)	5633	5545
Crystal size	0.1 × 0.02 × 0.01 mm	0.2 × 0.1 × 0.15 mm
Theta range for data collection	3.37 to 25.50°	3.35 to 26.00°
Limiting indices	-17 ≤ <i>h</i> ≤ 17, -24 ≤ <i>k</i> ≤ 21, -25 ≤ <i>l</i> ≤ 17	-14 ≤ <i>h</i> ≤ 14, -24 ≤ <i>k</i> ≤ 24, -19 ≤ <i>l</i> ≤ 29
Reflections collected / unique	34241 / 11112 [<i>R</i> _{int} = 0.0942]	25982 / 10891 [<i>R</i> _{int} = 0.1008]
Completeness to theta = 25.50	99.8 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.56973	1.00000 and 0.93287
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	11112 / 0 / 601	10891 / 0 / 647
Goodness-of-fit on <i>F</i> ²	1.003	0.956
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0545, <i>wR</i> ₂ = 0.0920	<i>R</i> ₁ = 0.0667, <i>wR</i> ₂ = 0.0930
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1069, <i>wR</i> ₂ = 0.1096	<i>R</i> ₁ = 0.1617, <i>wR</i> ₂ = 0.1188
Largest diff. peak and hole	3.442 and -1.820 e.Å ⁻³	1.925 and -1.763 e.Å ⁻³

Table S2. Selected bond lengths (Å) and bond angles (°) for **1** and **2**.

Complex 1			
Bond	Distance (Å)	Bond	Distance (Å)
Eu-O(21)	2.402(11)	W(9)-O(28)	1.731(13)
Eu-O(17)	2.405(12)	W(9)-O(21)	1.771(12)
Eu-O(18)	2.408(12)	W(9)-O(32)	2.161(11)
Eu-O(16)	2.428(11)	W(9)-O(27)	2.334(11)
Eu-O(22)	2.439(11)	W(10)-O(36)	1.752(13)
Eu-O(20)	2.445(12)	W(10)-O(34)	1.834(12)
Eu-W(9)	3.7783(12)	W(10)-O(32)	2.108(11)
Eu-W(2)	3.8261(13)	W(10)-O(27)	2.246(11)
Eu-W(5)	3.8347(13)	C(1)-N(4)	1.42(3)
Eu-W(6)	3.8376(13)	C(1)-C(2)	1.65(3)
W(1)-O(1)	1.732(14)	C(2)-C(3)	1.53(3)
W(1)-O(2)	1.842(11)	C(3)-N(3)	1.52(3)
W(1)-O(4)	2.126(12)	C(4)-N(3)	1.34(3)
W(1)-O(14)	2.243(12)	C(4)-C(7)	1.39(3)
W(2)-O(6)	1.734(12)	C(7)-C(8)	1.35(3)
W(2)-O(18)	1.765(12)	C(8)-C(9)	1.46(3)
W(2)-O(2)	2.075(12)	C(10)-C(13)	1.40(3)
W(2)-O(14)	2.379(11)	C(11)-C(12)	1.39(3)
W(3)-O(9)	1.696(12)	C(12)-N(2)	1.34(2)
W(3)-O(15)	1.777(12)	C(13)-N(2)	1.34(3)
W(3)-O(14)	2.317(12)	C(14)-C(15)	1.46(3)
W(4)-O(8)	1.739(11)	C(14)-N(2)	1.51(2)
W(4)-O(16)	1.785(12)	C(15)-C(16)	1.58(3)
W(4)-O(13)	1.931(12)	C(16)-N(1)	1.54(2)
W(4)-O(10)	1.941(13)	C(17)-C(17)#1	1.51(4)
W(4)-O(4)	2.139(12)	C(17)-N(5)	1.51(3)
W(4)-O(14)	2.304(11)	N(5)-C(18)	1.3900
W(4)-W(5)	3.2264(11)	N(5)-C(22)	1.3900
W(5)-O(7)	1.725(12)	C(18)-C(19)	1.3900
W(5)-O(17)	1.773(12)	C(20)-C(25)	1.42(2)
W(5)-O(13)	1.933(12)	C(28)-C(29)	1.50(3)
W(5)-O(12)	1.943(12)	C(28)-N(6)	1.53(2)
W(5)-O(3)	2.039(13)	C(23)-C(24)	1.3900
W(6)-O(31)	1.733(13)	C(23)-N(6)	1.3900
W(6)-O(19)	1.779(13)	C(24)-C(25)	1.3900
W(6)-O(35)	2.053(12)	C(25)-C(26)	1.3900
W(6)-O(27)	2.270(11)	C(26)-C(27)	1.3900
W(7)-O(30)	1.715(12)	C(27)-N(6)	1.3900
W(7)-O(20)	1.744(12)	C(29)-C(30)	1.42(4)
W(7)-O(27)	2.335(11)	C(30)-C(31)	1.40(4)
W(8)-O(29)	1.740(12)	C(31)-N(7)	1.52(3)
W(8)-O(22)	1.751(12)	N(7)-C(32)	1.3900
W(8)-O(23)	1.933(12)	N(7)-C(36)	1.3900
W(8)-O(24)	1.960(12)	C(32)-C(33)	1.3900
W(8)-O(33)	2.063(13)	C(34)-C(34)#2	1.51(3)
W(8)-O(27)	2.323(11)	C(35)-C(36)	1.3900
Angle	(°)	Angle	(°)

O(21)-Eu-O(17)	77.9(4)	O(25)-W(6)-O(27)	76.8(4)
O(21)-Eu-O(19)	73.8(4)	O(35)-W(6)-O(27)	71.9(4)
O(17)-Eu-O(19)	79.6(4)	O(31)-W(6)-Eu	133.2(4)
O(18)-Eu-O(19)	142.7(4)	O(19)-W(6)-Eu	28.3(4)
O(17)-Eu-O(15)	112.7(4)	O(25)-W(6)-Eu	85.5(3)
O(18)-Eu-O(15)	72.9(4)	O(35)-W(6)-Eu	129.9(3)
O(19)-Eu-O(15)	143.0(4)	O(27)-W(6)-Eu	58.0(3)
O(21)-Eu-O(16)	142.2(4)	O(30)-W(7)-O(20)	103.3(6)
O(17)-Eu-O(16)	71.6(4)	O(20)-W(7)-O(25)	92.1(5)
O(18)-Eu-O(16)	115.3(4)	O(25)-W(7)-O(24)	152.2(5)
O(19)-Eu-O(16)	79.0(4)	O(30)-W(7)-O(34)	96.8(5)
O(17)-Eu-O(22)	144.4(4)	O(20)-W(7)-O(34)	159.8(5)
O(18)-Eu-O(22)	77.8(4)	O(24)-W(7)-O(34)	81.4(5)
O(19)-Eu-O(22)	113.3(4)	O(30)-W(7)-O(27)	170.6(5)
O(17)-Eu-O(20)	142.2(4)	O(20)-W(7)-O(27)	86.0(5)
O(19)-Eu-O(20)	72.2(4)	O(34)-W(7)-O(27)	73.8(4)
O(22)-Eu-O(20)	71.7(4)	O(30)-W(7)-Eu	131.6(4)
O(21)-Eu-W(9)	21.3(3)	O(20)-W(7)-Eu	28.2(4)
O(17)-Eu-W(9)	95.3(3)	O(24)-W(7)-Eu	87.8(4)
O(18)-Eu-W(9)	92.0(3)	O(34)-W(7)-Eu	131.6(3)
O(19)-Eu-W(9)	64.8(3)	O(27)-W(7)-Eu	57.8(3)
O(16)-Eu-W(9)	143.4(3)	O(29)-W(8)-O(22)	103.5(6)
O(22)-Eu-W(9)	64.7(3)	O(22)-W(8)-O(23)	93.7(5)
O(17)-Eu-W(2)	64.7(3)	O(23)-W(8)-O(24)	152.8(5)
O(18)-Eu-W(2)	19.9(3)	O(29)-W(8)-O(33)	97.9(5)
O(15)-Eu-W(2)	64.1(3)	O(22)-W(8)-O(33)	158.5(5)
O(16)-Eu-W(2)	95.4(3)	O(23)-W(8)-O(33)	81.5(5)
W(9)-Eu-W(2)	109.99(3)	O(24)-W(8)-O(33)	83.3(5)
O(21)-Eu-W(5)	92.9(3)	O(29)-W(8)-O(27)	170.6(5)
O(17)-Eu-W(5)	19.9(3)	O(22)-W(8)-O(27)	85.8(5)
O(18)-Eu-W(5)	64.6(3)	O(23)-W(8)-O(27)	76.7(5)
O(19)-Eu-W(5)	96.3(3)	O(24)-W(8)-O(27)	77.4(4)
O(15)-Eu-W(5)	92.9(3)	O(33)-W(8)-O(27)	72.7(4)
O(16)-Eu-W(5)	64.2(3)	O(29)-W(8)-Eu	131.5(4)
W(9)-Eu-W(5)	112.41(3)	O(22)-W(8)-Eu	28.0(4)
W(2)-Eu-W(5)	50.62(2)	O(23)-W(8)-Eu	85.9(3)
O(21)-Eu-W(6)	65.4(3)	O(27)-W(8)-Eu	57.8(3)
O(17)-Eu-W(6)	95.9(3)	O(28)-W(9)-O(21)	105.4(6)
O(18)-Eu-W(6)	140.8(3)	O(28)-W(9)-O(23)	102.1(5)
O(19)-Eu-W(6)	20.4(3)	O(21)-W(9)-O(23)	95.9(5)
O(16)-Eu-W(6)	95.7(3)	O(23)-W(9)-O(26)	149.7(5)
O(20)-Eu-W(6)	64.0(3)	O(28)-W(9)-O(32)	92.9(5)
W(9)-Eu-W(6)	50.65(2)	O(21)-W(9)-O(32)	161.7(5)
W(2)-Eu-W(6)	153.14(3)	O(23)-W(9)-O(32)	81.4(5)
W(5)-Eu-W(6)	114.35(3)	O(26)-W(9)-O(32)	79.6(4)
O(1)-W(1)-O(2)	106.1(6)	O(28)-W(9)-O(27)	166.1(5)
O(2)-W(1)-O(5)	92.5(5)	O(21)-W(9)-O(27)	88.5(5)
O(1)-W(1)-O(3)	105.5(6)	O(26)-W(9)-O(27)	75.5(5)
O(2)-W(1)-O(3)	91.9(5)	O(32)-W(9)-O(27)	73.2(4)
O(5)-W(1)-O(3)	151.8(5)	O(28)-W(9)-Eu	134.9(4)
O(2)-W(1)-O(4)	155.7(5)	O(21)-W(9)-Eu	29.6(4)

O(5)-W(1)-O(4)	83.0(5)	O(23)-W(9)-Eu	87.8(3)
O(1)-W(1)-O(14)	172.7(5)	O(32)-W(9)-Eu	132.2(3)
O(2)-W(1)-O(14)	81.0(5)	O(27)-W(9)-Eu	59.0(3)
O(5)-W(1)-O(14)	77.8(5)	O(36)-W(10)-O(34)	104.3(6)
O(6)-W(2)-O(18)	104.4(5)	O(34)-W(10)-O(35)	91.4(5)
O(18)-W(2)-O(12)	93.7(5)	O(36)-W(10)-O(33)	100.9(6)
O(6)-W(2)-O(11)	103.3(5)	O(35)-W(10)-O(33)	152.5(5)
O(18)-W(2)-O(11)	93.3(5)	O(36)-W(10)-O(32)	98.6(5)
O(12)-W(2)-O(11)	150.0(5)	O(33)-W(10)-O(32)	83.4(5)
O(6)-W(2)-O(2)	95.8(5)	O(36)-W(10)-O(27)	174.6(5)
O(18)-W(2)-O(2)	159.8(5)	O(34)-W(10)-O(27)	81.1(5)
O(12)-W(2)-O(2)	81.7(5)	O(35)-W(10)-O(27)	75.9(5)
O(6)-W(2)-O(14)	169.1(5)	O(33)-W(10)-O(27)	77.8(5)
O(18)-W(2)-O(14)	86.5(5)	W(1)-O(2)-W(2)	114.6(6)
O(2)-W(2)-O(14)	73.3(4)	W(1)-O(4)-W(4)	110.9(5)
O(6)-W(2)-Eu	132.1(4)	W(1)-O(5)-W(3)	115.0(6)
O(18)-W(2)-Eu	27.7(4)	W(4)-O(13)-W(5)	113.2(6)
O(12)-W(2)-Eu	86.7(4)	W(1)-O(14)-W(5)	95.7(4)
O(2)-W(2)-Eu	132.1(3)	W(1)-O(14)-W(4)	101.2(4)
O(14)-W(2)-Eu	58.8(3)	W(5)-O(14)-W(4)	89.5(4)
O(9)-W(3)-O(15)	104.0(6)	W(1)-O(14)-W(3)	94.4(4)
O(15)-W(3)-O(11)	91.0(5)	W(5)-O(14)-W(3)	169.8(6)
O(9)-W(3)-O(10)	102.1(6)	W(4)-O(14)-W(3)	89.8(4)
O(15)-W(3)-O(10)	93.1(5)	W(1)-O(14)-W(2)	91.1(4)
O(11)-W(3)-O(10)	153.6(5)	W(4)-O(14)-W(2)	167.8(6)
O(9)-W(3)-O(5)	97.9(6)	W(3)-O(14)-W(2)	89.3(4)
O(15)-W(3)-O(5)	158.0(5)	W(4)-O(16)-Eu	130.9(6)
O(11)-W(3)-O(5)	83.0(5)	W(2)-O(18)-Eu	132.3(6)
O(9)-W(3)-O(14)	170.1(5)	W(6)-O(19)-Eu	131.4(6)
O(15)-W(3)-O(14)	85.9(5)	W(9)-O(21)-Eu	129.1(6)
O(5)-W(3)-O(14)	72.2(4)	W(9)-O(23)-W(8)	115.5(6)
O(9)-W(3)-Eu	131.6(4)	W(7)-O(24)-W(8)	114.0(6)
O(15)-W(3)-Eu	27.6(4)	W(10)-O(27)-W(6)	95.2(4)
O(11)-W(3)-Eu	85.3(4)	W(10)-O(27)-W(8)	93.8(4)
O(10)-W(3)-Eu	86.3(4)	W(6)-O(27)-W(8)	171.0(6)
O(8)-W(4)-O(16)	104.9(6)	W(10)-O(27)-W(9)	100.1(4)
O(16)-W(4)-O(13)	94.4(5)	W(6)-O(27)-W(9)	90.1(4)
O(8)-W(4)-O(10)	99.8(5)	W(8)-O(27)-W(9)	88.9(4)
O(13)-W(4)-O(10)	153.0(5)	W(9)-O(27)-W(7)	167.9(6)
O(16)-W(4)-O(4)	160.4(5)	W(10)-O(32)-W(9)	110.6(5)
O(13)-W(4)-O(4)	81.9(5)	W(10)-O(33)-W(8)	115.2(6)
O(8)-W(4)-O(14)	167.8(5)	W(10)-O(34)-W(7)	113.3(6)
O(16)-W(4)-O(14)	87.2(5)	W(10)-O(35)-W(6)	116.7(6)
O(4)-W(4)-O(14)	73.2(4)	N(4)-C(1)-C(2)	109.1(18)
O(8)-W(4)-W(5)	136.6(4)	C(3)-C(2)-C(1)	109(2)
O(16)-W(4)-W(5)	84.5(4)	N(3)-C(3)-C(2)	104(2)
O(13)-W(4)-W(5)	33.4(4)	N(3)-C(4)-C(7)	119(2)
O(10)-W(4)-W(5)	122.2(4)	N(3)-C(5)-C(6)	123(3)
O(4)-W(4)-W(5)	81.9(3)	C(5)-C(6)-C(8)	118(2)
O(14)-W(4)-W(5)	45.0(3)	C(8)-C(7)-C(4)	120(2)
O(8)-W(4)-Eu	133.4(5)	C(7)-C(8)-C(6)	118(2)

O(16)-W(4)-Eu	28.5(4)	C(7)-C(8)-C(9)	122.0(19)
O(4)-W(4)-Eu	131.9(3)	C(10)-C(9)-C(11)	115(2)
O(14)-W(4)-Eu	58.7(3)	C(10)-C(9)-C(8)	122.7(19)
W(5)-W(4)-Eu	65.04(2)	C(12)-C(11)-C(9)	120.4(19)
O(17)-W(5)-O(1)	92.4(5)	N(2)-C(12)-C(11)	121.6(19)
O(7)-W(5)-O(12)	99.9(6)	C(15)-C(14)-N(2)	109.0(16)
O(13)-W(5)-O(12)	154.7(5)	C(14)-C(15)-C(16)	107.3(17)
O(7)-W(5)-O(3)	98.1(6)	N(1)-C(16)-C(15)	104.3(16)
O(17)-W(5)-O(3)	158.4(5)	C(17)#1-C(17)-N(5)	120(2)
O(13)-W(5)-O(3)	82.8(5)	C(18)-N(5)-C(22)	120.0
O(12)-W(5)-O(3)	82.6(5)	C(18)-N(5)-C(17)	115.1(19)
O(7)-W(5)-O(14)	170.2(6)	C(22)-N(5)-C(17)	123.0(19)
O(17)-W(5)-O(14)	86.3(5)	N(5)-C(18)-C(19)	120.0
O(3)-W(5)-O(14)	72.1(5)	C(19)-C(20)-C(21)	120.0
O(7)-W(5)-W(4)	135.8(4)	C(19)-C(20)-C(25)	116(2)
O(17)-W(5)-W(4)	82.5(4)	C(21)-C(20)-C(25)	124(2)
O(13)-W(5)-W(4)	33.4(4)	C(21)-C(22)-N(5)	120.0
O(12)-W(5)-W(4)	123.6(4)	C(29)-C(28)-N(6)	118(2)
O(3)-W(5)-W(4)	81.9(4)	C(24)-C(25)-C(20)	119(2)
O(14)-W(5)-W(4)	45.6(3)	C(26)-C(25)-C(20)	121(2)
O(17)-W(5)-Eu	27.5(4)	N(6)-C(27)-C(26)	120.0
O(13)-W(5)-Eu	87.7(4)	C(27)-N(6)-C(23)	120.0
O(12)-W(5)-Eu	86.5(4)	C(27)-N(6)-C(28)	109.5(19)
O(3)-W(5)-Eu	131.0(4)	C(23)-N(6)-C(28)	129.4(19)
O(14)-W(5)-Eu	58.9(3)	C(30)-C(29)-C(28)	126(2)
W(4)-W(5)-Eu	65.25(2)	C(30)-C(31)-N(7)	118(2)
O(31)-W(6)-O(19)	104.9(5)	C(36)-N(7)-C(31)	117.6(17)
O(31)-W(6)-O(26)	101.5(6)	C(33)-C(32)-N(7)	120.0
O(19)-W(6)-O(26)	93.1(5)	C(32)-C(33)-C(34)	120.0
O(19)-W(6)-O(25)	91.4(5)	C(33)-C(34)-C(34)#2	107(3)
O(26)-W(6)-O(25)	153.0(5)	C(35)-C(34)-C(34)#2	132(3)
O(31)-W(6)-O(35)	97.0(5)	C(35)-C(36)-N(7)	120.0
O(19)-W(6)-O(35)	158.1(5)	C(12)-N(2)-C(13)	120.4(19)
O(26)-W(6)-O(35)	82.8(5)	C(12)-N(2)-C(14)	118.5(17)
O(31)-W(6)-O(27)	168.8(5)	C(13)-N(2)-C(14)	120.3(19)
O(19)-W(6)-O(27)	86.2(5)	C(5)-N(3)-C(3)	116(2)
O(26)-W(6)-O(27)	77.0(5)	C(4)-N(3)-C(3)	123(2)

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

Complex 2			
Bond	Distance (Å)	Bond	Distance (Å)
W(1)-O(19)	1.708(16)	W(9)-O(24)	2.177(14)
W(1)-O(22)	1.898(15)	W(10)-O(40)	1.730(16)
W(1)-O(13)	1.936(15)	W(10)-O(37)	1.912(16)
W(1)-O(23)	2.274(16)	W(10)-O(33)	1.947(14)
W(2)-O(12)	1.732(17)	W(10)-O(26)	2.185(14)
W(2)-O(5)	1.892(14)	W(11)-O(38)	1.699(15)
W(2)-O(21)	1.954(16)	W(11)-O(36)	1.883(17)
W(2)-O(23)	2.211(14)	W(11)-O(21)	1.932(17)
W(3)-O(4)	1.744(17)	W(11)-O(20)	1.973(19)

W(3)-O(9)	1.901(13)	W(11)-O(23)	2.217(14)
W(3)-O(3)	1.952(17)	W(12)-O(27)	1.692(17)
W(3)-O(8)	2.269(17)	W(12)-O(15)	1.918(15)
W(4)-O(1)	1.711(16)	W(12)-O(22)	1.932(13)
W(4)-O(3)	1.892(19)	W(12)-O(39)	1.949(17)
W(4)-O(5)	1.930(13)	W(12)-O(26)	2.248(16)
W(4)-O(7)	1.941(17)	OW3A-OW3B	1.64(7)
W(4)-O(8)	2.242(15)	OW4A-OW4B#1	1.75(10)
W(5)-O(11)	1.717(14)	OW4B-OW4A#1	1.75(10)
W(5)-O(16)	1.897(16)	C(1)-C(2)	1.35(5)
W(5)-O(18)	1.913(18)	C(1)-N(1)	1.48(4)
W(5)-O(2)	1.967(15)	C(2)-C(3)	1.41(4)
W(5)-O(8)	2.243(13)	C(3)-N(2)	1.45(3)
W(6)-O(10)	1.708(17)	C(4)-N(2)	1.34(4)
W(6)-O(14)	1.869(16)	C(4)-C(7)	1.40(4)
W(6)-O(25)	1.962(15)	C(5)-C(6)	1.32(4)
W(6)-O(24)	2.095(15)	C(5)-N(2)	1.35(3)
W(6)-W(7)	3.2186(14)	C(6)-C(8)	1.41(4)
W(7)-O(29)	1.705(16)	C(7)-C(8)	1.36(3)
W(7)-O(17)	1.888(15)	C(8)-C(9)	1.46(3)
W(7)-O(18)	1.909(16)	C(9)-C(10)	1.33(3)
W(7)-O(30)	1.949(17)	C(9)-C(11)	1.36(4)
W(7)-O(24)	2.201(13)	C(10)-C(13)	1.41(3)
W(8)-O(32)	1.694(13)	C(11)-C(12)	1.34(4)
W(8)-O(30)	1.861(18)	C(12)-N(3)	1.41(3)
W(8)-O(33)	1.913(15)	C(13)-N(3)	1.31(3)
W(8)-O(28)	1.962(17)	C(14)-C(15)	1.42(3)
W(8)-O(26)	2.196(13)	C(14)-N(3)	1.52(3)
W(9)-O(34)	1.706(18)	C(15)-C(16)	1.47(3)
W(9)-O(35)	1.897(18)	C(16)-N(4)	1.50(3)
W(9)-O(31)	1.924(15)		
Angle	(°)	Angle	(°)
O(19)-W(1)-O(22)	101.6(7)	O(16)-W(8)-O(26)	88.7(5)
O(22)-W(1)-O(9)	86.6(6)	O(28)-W(8)-O(26)	74.1(5)
O(19)-W(1)-O(20)	96.3(7)	O(34)-W(9)-O(35)	98.7(8)
O(22)-W(1)-O(20)	90.6(6)	O(35)-W(9)-O(25)	162.5(7)
O(9)-W(1)-O(20)	161.9(7)	O(34)-W(9)-O(31)	97.6(8)
O(22)-W(1)-O(13)	162.8(6)	O(35)-W(9)-O(31)	89.5(6)
O(20)-W(1)-O(13)	88.7(6)	O(25)-W(9)-O(31)	92.8(7)
O(19)-W(1)-O(23)	166.9(6)	O(34)-W(9)-O(36)	99.9(8)
O(9)-W(1)-O(23)	86.9(6)	O(35)-W(9)-O(36)	85.1(7)
O(13)-W(1)-O(23)	74.6(6)	O(31)-W(9)-O(36)	162.3(7)
O(12)-W(2)-O(5)	100.0(8)	O(34)-W(9)-O(24)	169.1(8)
O(12)-W(2)-O(21)	98.3(8)	O(25)-W(9)-O(24)	74.9(6)
O(5)-W(2)-O(21)	161.5(6)	O(36)-W(9)-O(24)	88.4(6)
O(5)-W(2)-O(13)	91.7(7)	O(34)-W(9)-W(6)	132.3(7)
O(21)-W(2)-O(13)	88.4(7)	O(35)-W(9)-W(6)	129.0(4)
O(12)-W(2)-O(14)	99.3(8)	O(25)-W(9)-W(6)	34.6(4)
O(5)-W(2)-O(14)	86.5(7)	O(31)-W(9)-W(6)	82.8(5)
O(13)-W(2)-O(14)	161.7(6)	O(36)-W(9)-W(6)	87.5(5)
O(12)-W(2)-O(23)	170.5(7)	O(24)-W(9)-W(6)	40.3(4)

O(13)-W(2)-O(23)	75.7(6)	O(40)-W(10)-O(37)	101.8(8)
O(14)-W(2)-O(23)	86.1(6)	O(40)-W(10)-O(39)	98.1(9)
O(4)-W(3)-O(9)	100.2(7)	O(37)-W(10)-O(39)	90.2(7)
O(9)-W(3)-O(15)	87.1(6)	O(37)-W(10)-O(35)	86.9(7)
O(4)-W(3)-O(6)	98.3(7)	O(39)-W(10)-O(35)	161.7(7)
O(9)-W(3)-O(6)	161.5(7)	O(40)-W(10)-O(33)	95.9(8)
O(9)-W(3)-O(3)	88.8(7)	O(37)-W(10)-O(33)	162.2(6)
O(15)-W(3)-O(3)	160.8(7)	O(35)-W(10)-O(33)	87.9(6)
O(4)-W(3)-O(8)	169.6(7)	O(40)-W(10)-O(26)	167.8(7)
O(9)-W(3)-O(8)	87.3(6)	O(39)-W(10)-O(26)	75.9(6)
O(6)-W(3)-O(8)	74.3(6)	O(35)-W(10)-O(26)	86.0(6)
O(1)-W(4)-O(3)	101.3(8)	O(38)-W(11)-O(36)	103.4(7)
O(3)-W(4)-O(2)	91.0(7)	O(38)-W(11)-O(21)	96.3(8)
O(1)-W(4)-O(5)	98.6(7)	O(36)-W(11)-O(21)	91.2(7)
O(3)-W(4)-O(5)	88.7(7)	O(37)-W(11)-O(21)	161.5(6)
O(2)-W(4)-O(5)	160.7(6)	O(38)-W(11)-O(20)	94.7(7)
O(3)-W(4)-O(7)	159.4(7)	O(37)-W(11)-O(20)	87.6(7)
O(2)-W(4)-O(7)	89.1(7)	O(21)-W(11)-O(20)	89.3(7)
O(5)-W(4)-O(7)	84.5(7)	O(38)-W(11)-O(23)	166.4(7)
O(1)-W(4)-O(8)	173.5(7)	O(36)-W(11)-O(23)	86.9(6)
O(2)-W(4)-O(8)	74.7(6)	O(21)-W(11)-O(23)	74.3(6)
O(5)-W(4)-O(8)	86.6(6)	O(20)-W(11)-O(23)	75.6(6)
O(11)-W(5)-O(16)	102.0(7)	O(27)-W(12)-O(28)	99.0(7)
O(11)-W(5)-O(18)	100.2(7)	O(27)-W(12)-O(15)	102.1(7)
O(16)-W(5)-O(18)	87.8(7)	O(28)-W(12)-O(22)	160.7(7)
O(11)-W(5)-O(6)	99.5(7)	O(15)-W(12)-O(22)	85.7(6)
O(18)-W(5)-O(6)	160.3(5)	O(27)-W(12)-O(39)	96.3(8)
O(16)-W(5)-O(2)	160.2(6)	O(28)-W(12)-O(39)	90.3(7)
O(18)-W(5)-O(2)	87.4(7)	O(22)-W(12)-O(39)	88.2(6)
O(11)-W(5)-O(8)	168.8(6)	O(27)-W(12)-O(26)	167.5(6)
O(18)-W(5)-O(8)	86.4(6)	O(28)-W(12)-O(26)	73.9(6)
O(6)-W(5)-O(8)	74.0(6)	O(22)-W(12)-O(26)	87.2(6)
O(10)-W(6)-O(7)	100.6(8)	W(4)-O(2)-W(5)	117.3(8)
O(14)-W(6)-O(7)	88.1(7)	W(2)-O(5)-W(4)	152.1(9)
O(10)-W(6)-O(25)	94.9(8)	W(6)-O(7)-W(4)	150.3(9)
O(7)-W(6)-O(25)	164.5(7)	W(4)-O(8)-W(5)	94.7(6)
O(10)-W(6)-O(17)	91.7(7)	W(4)-O(8)-W(3)	93.9(5)
O(14)-W(6)-O(17)	166.7(7)	W(1)-O(13)-W(2)	115.4(7)
O(7)-W(6)-O(17)	88.5(6)	W(5)-O(16)-W(8)	147.7(8)
O(14)-W(6)-O(24)	91.3(7)	W(7)-O(17)-W(6)	111.5(8)
O(7)-W(6)-O(24)	89.0(6)	W(1)-O(20)-W(11)	115.0(8)
O(25)-W(6)-O(24)	75.9(6)	W(2)-O(23)-W(11)	95.9(5)
O(10)-W(6)-W(9)	127.4(6)	W(11)-O(23)-W(1)	94.2(6)
O(7)-W(6)-W(9)	131.2(5)	W(6)-O(24)-W(9)	97.5(5)
O(25)-W(6)-W(9)	33.7(5)	W(9)-O(24)-W(7)	96.1(6)
O(17)-W(6)-W(9)	82.7(4)	W(9)-O(25)-W(6)	111.7(7)
O(24)-W(6)-W(9)	42.2(4)	W(12)-O(28)-W(8)	116.5(7)
O(10)-W(6)-W(7)	124.5(5)	W(8)-O(30)-W(7)	153.8(9)
O(14)-W(6)-W(7)	133.8(6)	W(9)-O(31)-W(7)	115.4(9)
O(7)-W(6)-W(7)	86.9(4)	W(9)-O(35)-W(10)	150.8(9)
O(25)-W(6)-W(7)	84.5(4)	W(11)-O(36)-W(9)	151.1(9)

O(17)-W(6)-W(7)	33.1(5)	W(10)-O(37)-W(11)	149.4(9)
W(9)-W(6)-W(7)	60.82(3)	C(2)-C(1)-N(1)	122(4)
O(17)-W(7)-O(18)	92.4(7)	C(1)-C(2)-C(3)	121(4)
O(29)-W(7)-O(31)	95.1(7)	C(2)-C(3)-N(2)	111(3)
O(17)-W(7)-O(31)	90.8(6)	N(2)-C(4)-C(7)	124(3)
O(18)-W(7)-O(31)	162.4(7)	C(6)-C(5)-N(2)	117(3)
O(29)-W(7)-O(30)	99.6(7)	C(5)-C(6)-C(8)	125(3)
O(18)-W(7)-O(30)	83.9(7)	C(8)-C(7)-C(4)	116(3)
O(31)-W(7)-O(30)	87.8(6)	C(7)-C(8)-C(6)	117(3)
O(29)-W(7)-O(24)	167.1(7)	C(7)-C(8)-C(9)	120(3)
O(17)-W(7)-O(24)	75.6(6)	C(6)-C(8)-C(9)	123(2)
O(18)-W(7)-O(24)	90.1(6)	C(10)-C(9)-C(11)	115(3)
O(31)-W(7)-O(24)	74.0(6)	C(10)-C(9)-C(8)	124(3)
O(29)-W(7)-W(6)	133.1(6)	C(11)-C(9)-C(8)	121(2)
O(17)-W(7)-W(6)	35.4(4)	C(9)-C(10)-C(13)	126(3)
O(18)-W(7)-W(6)	90.1(4)	C(12)-C(11)-C(9)	122(2)
O(30)-W(7)-W(6)	127.0(4)	C(11)-C(12)-N(3)	119(3)
O(24)-W(7)-W(6)	40.2(4)	N(3)-C(13)-C(10)	115.8(19)
O(32)-W(8)-O(30)	103.0(7)	C(15)-C(14)-N(3)	115(2)
O(32)-W(8)-O(33)	98.5(7)	C(14)-C(15)-C(16)	117(3)
O(30)-W(8)-O(33)	92.3(7)	C(15)-C(16)-N(4)	113(2)
O(30)-W(8)-O(16)	86.1(7)	C(4)-N(2)-C(5)	120(3)
O(33)-W(8)-O(16)	162.7(6)	C(4)-N(2)-C(3)	120(3)
O(32)-W(8)-O(28)	96.4(7)	C(5)-N(2)-C(3)	119(3)
O(30)-W(8)-O(28)	160.2(6)	C(13)-N(3)-C(12)	121(2)
O(33)-W(8)-O(28)	88.7(7)	C(13)-N(3)-C(14)	124.6(19)
O(33)-W(8)-O(26)	74.0(6)	C(12)-N(3)-C(14)	114(2)

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

Table S3. Hydrogen bond distances (Å) and angles (°). (D, donor atom; A, acceptor atom) for **1** and **2**.

Complex 1				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<DHA
N(1)-H(1C)···O(30)#1	0.89	2.42	2.8595(1)	111
N(1)-H(1D)···Ow(1)	0.89	2.02	2.7656(1)	141
N(1)-H(1D)···O(30)#1	0.89	2.56	2.8595(1)	100
N(1)-H(1E)···O(3)	0.89	1.84	2.7205(1)	172
N(4)-H(4A)···Ow(2)#6	0.89	1.99	2.8728(1)	171
N(4)-H(4B)···O(5)#6	0.89	1.99	2.8010(1)	151
N(4)-H(4C)···O(33)#3	0.89	2.04	2.8157(1)	145
C(1)-H(1B)···O(6)#7	0.97	2.26	3.1174(1)	147
C(2)-H(2B)···O(26)#2	0.97	2.48	3.3099(1)	144
C(3)-H(3A)···O(9)#6	0.97	2.37	3.3263(1)	169
C(3)-H(3B)···O(36)#3	0.97	2.49	3.4105(1)	158
C(4)-H(4)···O(34)#3	0.93	2.47	3.3635(1)	160
C(5)-H(5)···O(17)#2	0.93	2.48	3.0747(1)	122
C(6)-H(6)···O(17)#2	0.93	2.50	3.0730(1)	120
C(11)-H(11)···O(8)	0.93	2.51	3.1060(1)	122
C(13)-H(13)···O(29)#1	0.93	2.50	3.2213(1)	135
C(13)-H(13)···O(6) #2	0.93	2.45	3.1755(1)	135
C(14)-H(14B)···O(26)#5	0.97	2.47	3.2545(1)	138
C(14)-H(14B)···O(32)#5	0.97	2.56	3.4533(1)	152
C(14)-H(14B)···O(35)#5	0.97	2.40	3.1636(1)	135
C(15)-H(15A)···Ow(1)	0.97	2.48	3.1882(1)	130
C(16)-H(16A)···O(24)#1	0.97	2.40	3.0442(1)	124
C(17)-H(17B)···O(22)#1	0.97	2.37	3.2423(1)	149
C(18)-H(18)···O(23)#2	0.93	2.04	2.6482(1)	121
C(18)-H(18)···O(29)#2	0.93	2.55	3.4329(1)	158
C(22)-H(22)···O(22)#1	0.93	2.17	2.9906(1)	146
C(24)-H(24)···O(28)#2	0.93	2.11	3.0379(1)	173
C(27)-H(27)···O(16)	0.93	2.35	2.7980(1)	109
C(27)-H(27)···O(19)	0.93	2.17	3.0504(1)	158
C(28)-H(28A)···O(16)	0.97	2.20	2.9175(1)	130
C(28)-H(28A)···O(20)	0.97	2.53	3.3153(1)	138
C(29)-H(29A)···O(30)#3	0.97	2.27	3.1944(1)	160
C(29)-H(29B)···N(7)	0.97	2.58	2.9292(1)	102
C(30)-H(30B)···O(30)	0.97	2.56	3.4433(1)	152
C(31)-H(31A)···Ow(3)#4	0.97	2.56	3.2020(1)	124
C(31)-H(31B)···O(7) #4	0.97	2.38	3.3470(1)	171
C(32)-H(32)···O(25)#3	0.93	2.35	3.2032(1)	153
C(32)-H(32)···O(34)#3	0.93	2.48	2.9723(1)	113
C(32)-H(32)···O(35)#3	0.93	2.47	3.2307(1)	139
C(33)-H(33)···O(36)#3	0.93	2.46	3.3587(1)	163
C(35)-H(35)···O(36)#5	0.93	2.34	3.2697(1)	176
C(36)-H(36)···O(10)	0.93	2.26	3.0383(1)	140

Symmetry codes: #1, 3/2-x,1/2+y,1/2-z; #2, -1/2+x,1/2-y,1/2+z; #3, 2-x,-y,1-z; #4, 3/2-x,-1/2+y,1/2-z; #5, -1+x,y,z; #6, 1-x,-y,1-z; #7, x,y,1+z.

Complex 2				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<DHA

N(1)-H(1C)···O(38)#5	0.89	2.57	3.3151(2)	142
N(1)-H(1D)···O(15)#3	0.89	2.56	3.4100(3)	161
N(1)-H(1D)···O(28)#3	0.89	2.39	2.9698(2)	123
N(1)-H(1E)···O(10)#2	0.89	2.18	3.0468(2)	164
N(1)-H(1E)···O(17)#2	0.89	2.36	2.9483(2)	123
N(4)-H(4A)···Ow(2)	0.89	1.95	2.7859(2)	155
N(4)-H(4B)···O(11)	0.89	2.15	2.9186(2)	145
N(4)-H(4B)···O(21)#4	0.89	2.47	3.0294(2)	121
N(4)-H(4C)···O(14)#4	0.89	2.51	3.1031(2)	125
N(4)-H(4C)···O(25)#4	0.89	2.52	3.3383(2)	154
C(1)-H(1A)···O(20)#5	0.97	2.34	3.2857(2)	166
C(1)-H(1B)···O(6)#3	0.97	2.49	3.2833(2)	139
C(2)-H(2A)···O(25)#2	0.97	2.59	3.5221(3)	162
C(2)-H(2A)···O(31)#2	0.97	2.56	3.2764(2)	130
C(3)-H(3B)···Ow(1)#2	0.97	2.60	3.3609(3)	136
C(4)-H(4)···O(12)#5	0.93	2.60	3.1259(2)	117
C(4)-H(4)···O(13)#5	0.93	2.46	3.3079(2)	151
C(5)-H(5)···Ow(1 #2	0.93	2.30	3.1701(2)	156
C(7)-H(7)···O(12)#5	0.93	2.42	3.0162(2)	122
C(10)-H(10)···O(4)#1	0.93	2.48	3.0993(2)	124
C(12)-H(12)···O(34)#4	0.93	2.35	2.9633(2)	123
C(13)-H(13)···O(29)	0.93	2.40	3.1837(2)	142
C(13)-H(13)···O(4)#1	0.93	2.55	3.1014(2)	119
C(14)-H(14A)···O(32)	0.97	2.58	3.1525(2)	118
C(14)-H(14B)···O(29)	0.97	2.40	3.2407(2)	145
C(16)-H(16A)···O(19)#1	0.97	2.44	3.4072(3)	171

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