Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

Assembly of the first polyoxometalates-based hybrid with [ring+helix] channels and Photocatalytic Activity

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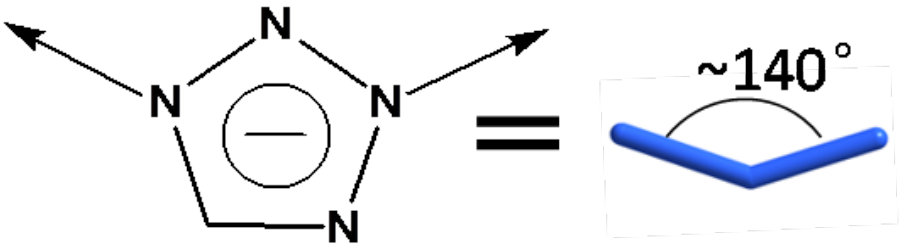
Fig.S1 The representation of tetrazolate ring as bent linkers.



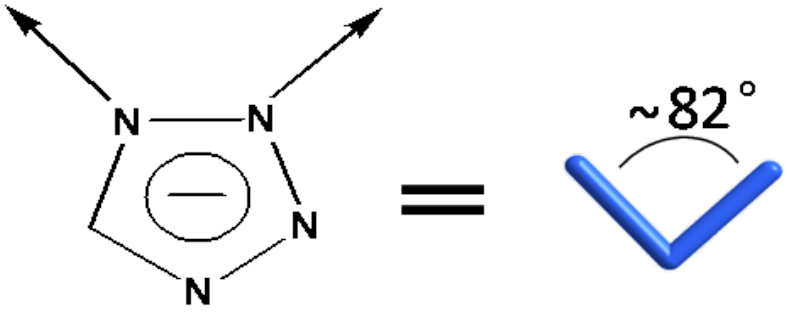


Fig.S2. The simulative and experimental powder X-ray diffraction patterns of the title compound.

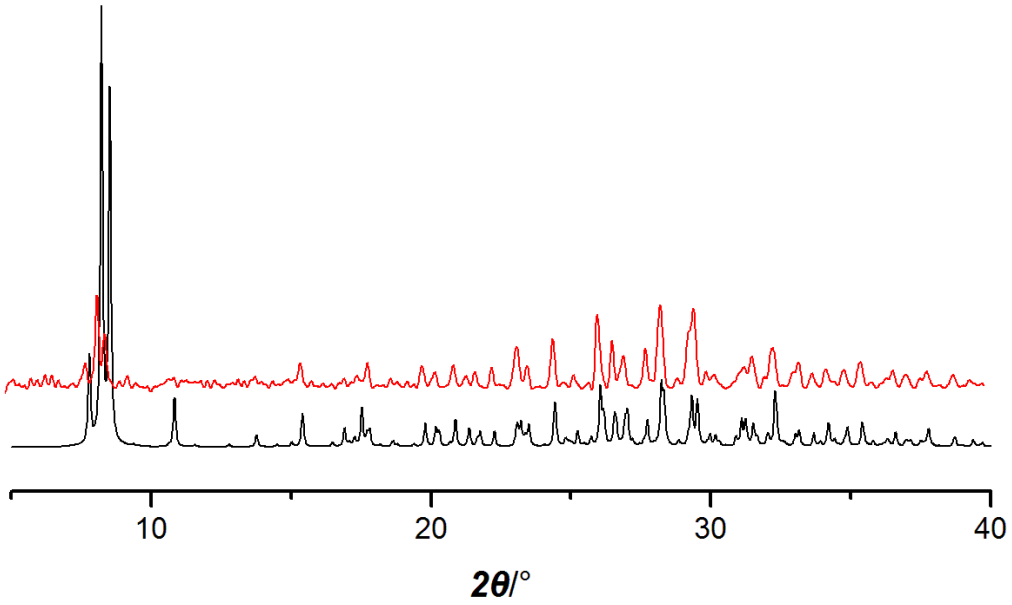


Fig.S3. IR spectrum of the title compound.

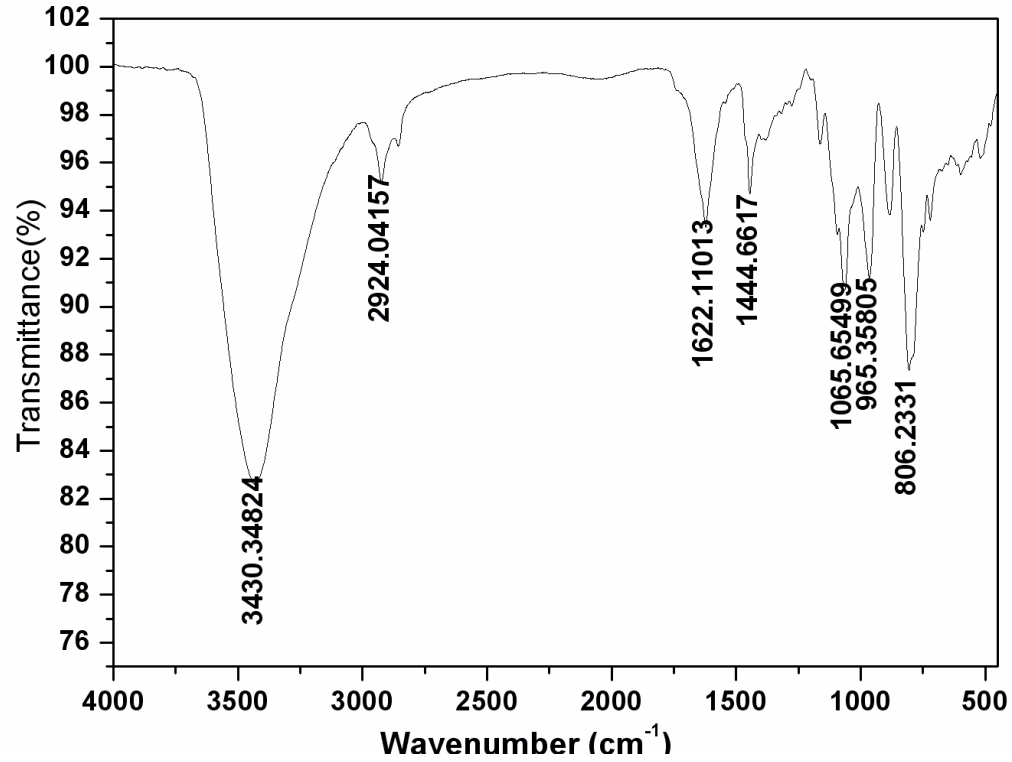


Table S1. Crystal Data and Structure Refinements for the new compound

Compound	**1**
Formula	C24H16N20K2Ag6PW12O40
CCDC	840486
Fw	4187
T (K)	296(2)
space group	$P2_1/c$
a (Å)	10.5554(8)
b (Å)	22.6863(18)
c (Å)	12.4204(10)
α (°)	90
β (°)	100.712(15)
γ (°)	90
V (Å^3)	2922.4(3)
Z	2
D_c (g·cm^{-3})	4.758
μ (mm^{-1})	25.749
F(000)	3686
final*R*1[a], *wR*2[b] [$I > 2\sigma(I)$]	0.0582, 0.1408
final*R*1[a], *wR*2[b] (all data)	0.0817, 0.1532
GOF on F^2	1.042

[a] $R_1=\sum \| F_o \| - | F_c \| / \sum | F_o |$. [b] $wR_2 = \{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

Table S2. Bond lengths [Å] and angles [°] for the title compound.

N(9)-Ag(3)#1	2.303(16)	O(96)-O(23)#5	1.57(3)
N(10)-Ag(3)	2.215(16)	N(7)-Ag(2)#2	2.168(16)
N(1)-Ag(1)	2.329(16)	N(2)-Ag(1)	2.248(17)
N(3)-Ag(2)	2.175(15)	O(8)-W(4)#5	1.84(2)
N(6)-Ag(3)#3	2.356(17)	O(99)-W(5)#5	2.516(13)
O(2)-K(1)#4	2.81(2)	O(19)-W(3)	1.879(14)
O(7)-W(6)	1.869(18)	O(20)-W(2)#5	1.905(16)
O(10)-W(6)	1.672(15)	O(98)-K(1)#1	2.72(2)
O(10)-Ag(1)	2.470(15)	P(2)-O(23)#5	1.448(14)
O(11)-W(6)	1.879(17)	P(2)-O(96)#5	1.539(13)

O(11)-W(1)	1.883(17)	P(2)-O(1)#5	1.540(13)
O(12)-W(3)	1.867(15)	P(2)-O(99)#5	1.571(16)
O(12)-W(2)#5	1.891(14)	Ag(1)-O(14)#6	2.535(17)
O(13)-W(3)	1.660(15)	Ag(1)-Ag(2)	3.196(2)
O(14)-W(1)	1.666(16)	Ag(2)-N(7)#7	2.168(16)
O(14)-Ag(1)#1	2.535(17)	Ag(3)-N(9)#6	2.303(16)
O(14)-K(1)#1	3.217(17)	Ag(3)-N(6)#8	2.356(17)
O(15)-W(5)	1.882(13)	Ag(3)-K(1)#8	3.695(5)
O(15)-W(1)#5	1.894(13)	W(1)-O(15)#5	1.894(13)
W(2)-O(23)#5	2.442(13)	W(1)-K(1)#1	3.807(5)
W(2)-K(1)#1	3.790(5)	W(2)-O(12)#5	1.891(14)
W(4)-O(8)#5	1.84(2)	W(2)-O(20)#5	1.905(16)
O(23)-O(96)#5	1.57(3)	W(5)-O(99)#5	2.516(13)
O(23)-O(99)	1.6941	K(1)-C(8)#3	2.71(2)
O(23)-W(2)#5	2.442(13)	K(1)-C(12)#3	2.71(3)
O(23)-W(3)	2.516(13)	K(1)-O(98)#6	2.72(2)
O(23)-W(4)	2.523(16)	K(1)-O(2)#9	2.81(2)
K(1)-O(14)#6	3.217(17)	C(12)-K(1)#8	2.71(3)
K(1)-O(18)#6	3.23(2)	C(10)-N(6)-N(4)	107.3(17)
K(1)-Ag(3)#3	3.695(5)	C(10)-N(6)-Ag(3)#3	132.0(14)
C(7)-K(1)#2	2.98(3)	N(4)-N(6)-Ag(3)#3	120.6(14)
C(8)-K(1)#8	2.71(2)	C(10)-N(6)-K(1)	142.1(13)
C(11)-K(1)#2	2.82(3)	N(4)-N(6)-K(1)	43.8(11)
Ag(1)-N(2)-K(1)	97.2(6)	Ag(3)#3-N(6)-K(1)	81.8(6)
W(4)-O(2)-K(1)#4	142.4(11)	W(4)-O(5)-W(1)	137.0(14)
W(6)-O(10)-Ag(1)	156.1(10)	W(6)-O(7)-W(2)	139.5(11)
W(6)-O(11)-W(1)	139.6(11)	W(4)#5-O(8)-W(5)	141.3(13)
W(1)-O(14)-Ag(1)#1	146.5(9)	W(3)-O(12)-W(2)#5	138.4(9)
W(5)-O(15)-W(1)#5	138.3(8)	Ag(1)#1-O(14)-K(1)#1	96.4(5)
W(3)-O(1)-W(6)	93.4(5)	P(2)-O(1)-W(3)	129.4(8)
P(2)-O(1)-W(5)	120.6(8)	O(23)-O(1)-W(3)	75.9(3)
O(23)-O(1)-W(5)	132.7(3)	P(2)-O(1)-W(6)	120.1(7)
W(3)-O(1)-W(5)	93.6(4)	O(23)-O(1)-W(6)	135.7(4)
N(1)-N(9)-Ag(3)#1	128.0(12)	P(2)-O(23)-O(96)#5	61.2(9)
C(2)-N(9)-Ag(3)#1	123.1(13)	P(2)-O(23)-O(1)	58.8(5)
O(96)#5-O(23)-O(99)	100.3(9)	O(96)#5-O(23)-O(1)	96.2(10)
O(1)-O(23)-O(99)	94.1	P(2)-O(23)-O(99)	59.4(6)
C(11)-N(7)-Ag(2)#2	122.7(15)	P(2)-O(23)-W(2)#5	128.4(8)
C(8)-N(7)-Ag(2)#2	118.7(14)	O(96)#5-O(23)-W(2)#5	67.2(9)
N(2)-N(5)-C(10)	105.0(18)	O(1)-O(23)-W(2)#5	130.3(3)
O(99)-O(23)-W(2)#5	133.8(3)	O(96)#5-P(2)-O(1)#5	77.0(6)
P(2)-O(23)-W(3)	122.8(7)	O(96)-P(2)-O(1)#5	103.0(6)
O(96)#5-O(23)-W(3)	129.6(12)	O(23)-P(2)-O(1)	67.7(6)
O(1)-O(23)-W(3)	64.1(3)	O(23)#5-P(2)-O(1)	112.3(6)

O(99)-O(23)-W(3)	125.5(3)	O(96)#5-P(2)-O(1)	103.0(6)
W(2)#5-O(23)-W(3)	90.2(4)	O(96)-P(2)-O(1)	77.0(6)
P(2)-O(23)-W(4)	124.3(8)	O(1)#5-P(2)-O(1)	180.0
O(96)#5-O(23)-W(4)	133.3(12)	O(23)-P(2)-O(99)	68.1(7)
O(1)-O(23)-W(4)	127.4(3)	O(23)#5-P(2)-O(99)	111.9(7)
O(99)-O(23)-W(4)	64.9(3)	O(96)#5-P(2)-O(99)	107.4(6)
W(2)#5-O(23)-W(4)	91.0(5)	O(96)-P(2)-O(99)	72.6(6)
W(3)-O(23)-W(4)	88.9(5)	O(1)#5-P(2)-O(99)	75.5(9)
P(2)-O(96)-O(23)#5	55.6(8)	O(1)-P(2)-O(99)	104.5(9)
P(2)-O(96)-W(2)	130.2(8)	O(23)-P(2)-O(99)#5	111.9(7)
O(23)#5-O(96)-W(2)	74.6(10)	O(23)#5-P(2)-O(99)#5	68.1(7)
P(2)-O(96)-W(1)	121.2(8)	O(96)#5-P(2)-O(99)#5	72.6(6)
O(23)#5-O(96)-W(1)	137.0(12)	O(96)-P(2)-O(99)#5	107.4(6)
W(2)-O(96)-W(1)	94.3(5)	O(1)#5-P(2)-O(99)#5	104.5(9)
P(2)-O(99)-O(23)	52.5(5)	O(1)-P(2)-O(99)#5	75.5(9)
P(2)-O(99)-W(4)	127.2(7)	O(99)-P(2)-O(99)#5	180.0(7)
O(23)-O(99)-W(4)	74.7(3)	N(2)-Ag(1)-N(1)	155.2(6)
P(2)-O(99)-W(1)	121.9(7)	N(2)-Ag(1)-O(10)	109.0(6)
O(23)-O(99)-W(1)	137.0(3)	N(1)-Ag(1)-O(10)	95.7(6)
W(4)-O(99)-W(1)	94.9(5)	N(2)-Ag(1)-O(14)#6	97.8(6)
P(2)-O(99)-W(5)#5	119.4(7)	N(1)-Ag(1)-O(14)#6	78.7(5)
O(23)-O(99)-W(5)#5	130.3(3)	O(10)-Ag(1)-O(14)#6	92.4(6)
W(4)-O(99)-W(5)#5	93.4(5)	N(2)-Ag(1)-Ag(2)	92.7(5)
W(1)-O(99)-W(5)#5	91.2(5)	N(1)-Ag(1)-Ag(2)	62.5(4)
W(5)-O(16)-W(6)	137.1(10)	O(10)-Ag(1)-Ag(2)	157.7(4)
W(2)-O(18)-K(1)#1	96.7(7)	O(14)#6-Ag(1)-Ag(2)	79.0(4)
W(3)-O(19)-W(4)	139.5(9)	N(7)#7-Ag(2)-N(3)	163.0(6)
W(4)-O(20)-W(2)#5	139.9(9)	N(7)#7-Ag(2)-Ag(1)	95.4(4)
W(6)-O(22)-W(3)	140.7(14)	N(3)-Ag(2)-Ag(1)	67.8(4)
W(2)-O(98)-W(1)	137.7(12)	N(10)-Ag(3)-N(9)#6	138.4(6)
W(2)-O(98)-K(1)#1	110.0(9)	N(10)-Ag(3)-N(6)#8	123.7(6)
W(1)-O(98)-K(1)#1	109.6(8)	N(9)#6-Ag(3)-N(6)#8	97.8(6)
O(23)-P(2)-O(23)#5	180.0(10)	N(10)-Ag(3)-K(1)#8	94.4(4)
O(23)-P(2)-O(96)#5	63.2(10)	N(9)#6-Ag(3)-K(1)#8	105.9(4)
O(23)#5-P(2)-O(96)#5	116.8(10)	N(6)#8-Ag(3)-K(1)#8	59.1(5)
O(23)-P(2)-O(96)	116.8(10)	O(14)-W(1)-O(11)	101.4(9)
O(23)#5-P(2)-O(96)	63.2(10)	O(14)-W(1)-O(15)#5	99.8(8)
O(96)#5-P(2)-O(96)	180.0(9)	O(11)-W(1)-O(15)#5	158.6(8)
O(23)-P(2)-O(1)#5	112.3(5)	O(14)-W(1)-O(98)	99.2(9)
O(23)#5-P(2)-O(1)#5	67.7(5)	O(11)-W(1)-O(98)	85.9(8)
O(15)#5-W(1)-O(98)	87.9(7)	O(18)-W(2)-K(1)#1	57.7(7)
O(14)-W(1)-O(5)	101.6(9)	O(98)-W(2)-K(1)#1	42.4(7)
O(11)-W(1)-O(5)	90.7(9)	O(12)#5-W(2)-K(1)#1	95.9(5)
O(15)#5-W(1)-O(5)	87.7(7)	O(20)#5-W(2)-K(1)#1	160.6(5)

O(98)-W(1)-O(5)	159.2(10)	O(7)-W(2)-K(1)#1	98.0(6)
O(14)-W(1)-O(99)	158.4(7)	O(96)-W(2)-K(1)#1	106.8(4)
O(11)-W(1)-O(99)	94.3(8)	O(23)#5-W(2)-K(1)#1	134.1(4)
O(15)#5-W(1)-O(99)	66.1(6)	O(13)-W(3)-O(12)	100.9(8)
O(98)-W(1)-O(99)	96.7(7)	O(13)-W(3)-O(19)	101.2(8)
O(5)-W(1)-O(99)	63.0(8)	O(12)-W(3)-O(19)	90.1(6)
O(14)-W(1)-O(96)	157.2(7)	O(13)-W(3)-O(22)	103.0(10)
O(11)-W(1)-O(96)	66.3(7)	O(12)-W(3)-O(22)	156.1(9)
O(15)#5-W(1)-O(96)	92.7(5)	O(19)-W(3)-O(22)	84.9(8)
O(98)-W(1)-O(96)	62.1(7)	O(13)-W(3)-O(9)	104.3(10)
O(5)-W(1)-O(96)	97.8(8)	O(12)-W(3)-O(9)	86.9(8)
O(99)-W(1)-O(96)	44.2(3)	O(19)-W(3)-O(9)	154.5(9)
O(14)-W(1)-K(1)#1	56.9(6)	O(22)-W(3)-O(9)	87.6(8)
O(11)-W(1)-K(1)#1	94.8(7)	O(13)-W(3)-O(1)	161.3(7)
O(15)#5-W(1)-K(1)#1	94.4(4)	O(12)-W(3)-O(1)	92.7(6)
O(98)-W(1)-K(1)#1	42.3(7)	O(19)-W(3)-O(1)	91.5(6)
O(5)-W(1)-K(1)#1	158.5(8)	O(22)-W(3)-O(1)	64.1(8)
O(99)-W(1)-K(1)#1	136.9(4)	O(9)-W(3)-O(1)	63.4(8)
O(96)-W(1)-K(1)#1	103.4(3)	O(13)-W(3)-O(23)	158.7(7)
O(18)-W(2)-O(98)	100.0(10)	O(12)-W(3)-O(23)	64.5(5)
O(18)-W(2)-O(12)#5	103.5(8)	O(19)-W(3)-O(23)	65.2(6)
O(98)-W(2)-O(12)#5	88.6(7)	O(22)-W(3)-O(23)	92.3(8)
O(18)-W(2)-O(20)#5	102.9(8)	O(9)-W(3)-O(23)	90.8(9)
O(98)-W(2)-O(20)#5	157.0(9)	O(1)-W(3)-O(23)	40.0(2)
O(12)#5-W(2)-O(20)#5	88.1(7)	O(2)-W(4)-O(8)#5	101.9(11)
O(18)-W(2)-O(7)	100.7(9)	O(2)-W(4)-O(20)	104.0(9)
O(98)-W(2)-O(7)	88.4(8)	O(8)#5-W(4)-O(20)	88.9(8)
O(12)#5-W(2)-O(7)	155.8(8)	O(2)-W(4)-O(5)	98.9(11)
O(20)#5-W(2)-O(7)	85.4(7)	O(8)#5-W(4)-O(5)	86.4(9)
O(18)-W(2)-O(96)	158.8(8)	O(20)-W(4)-O(5)	157.1(10)
O(98)-W(2)-O(96)	65.3(8)	O(2)-W(4)-O(19)	102.9(9)
O(12)#5-W(2)-O(96)	91.8(6)	O(8)#5-W(4)-O(19)	154.8(10)
O(20)#5-W(2)-O(96)	92.1(6)	O(20)-W(4)-O(19)	89.4(7)
O(7)-W(2)-O(96)	65.2(7)	O(5)-W(4)-O(19)	85.5(8)
O(18)-W(2)-O(23)#5	162.9(7)	O(2)-W(4)-O(99)	158.3(8)
O(98)-W(2)-O(23)#5	93.3(8)	O(8)#5-W(4)-O(99)	64.6(8)
O(12)#5-W(2)-O(23)#5	66.0(6)	O(20)-W(4)-O(99)	93.1(6)
O(20)#5-W(2)-O(23)#5	64.7(6)	O(5)-W(4)-O(99)	64.7(9)
O(7)-W(2)-O(23)#5	90.2(7)	O(19)-W(4)-O(99)	90.4(6)
O(96)-W(2)-O(23)#5	38.2(7)	O(2)-W(4)-O(23)	161.3(8)
O(8)#5-W(4)-O(23)	91.9(9)	N(4)-K(1)-O(98)#6	132.9(6)
O(20)-W(4)-O(23)	63.3(6)	C(8)#3-K(1)-O(98)#6	83.6(6)
O(5)-W(4)-O(23)	94.4(9)	C(12)#3-K(1)-O(98)#6	103.3(7)
O(19)-W(4)-O(23)	65.0(6)	N(4)-K(1)-O(2)#9	115.1(6)

O(99)-W(4)-O(23)	40.4(3)	C(8)#3-K(1)-O(2)#9	95.5(6)
O(21)-W(5)-O(9)	104.5(9)	C(12)#3-K(1)-O(2)#9	69.2(6)
O(21)-W(5)-O(15)	103.2(7)	O(98)#6-K(1)-O(2)#9	111.7(6)
O(9)-W(5)-O(15)	88.1(8)	N(4)-K(1)-C(11)#7	88.4(8)
O(21)-W(5)-O(16)	100.3(9)	C(8)#3-K(1)-C(11)#7	159.7(7)
O(9)-W(5)-O(16)	89.3(9)	C(12)#3-K(1)-C(11)#7	170.8(8)
O(15)-W(5)-O(16)	156.2(8)	O(98)#6-K(1)-C(11)#7	85.1(7)
O(21)-W(5)-O(8)	101.9(9)	O(2)#9-K(1)-C(11)#7	104.4(6)
O(9)-W(5)-O(8)	153.6(10)	N(4)-K(1)-C(7)#7	88.3(7)
O(15)-W(5)-O(8)	86.0(7)	C(8)#3-K(1)-C(7)#7	170.8(7)
O(16)-W(5)-O(8)	86.0(10)	C(12)#3-K(1)-C(7)#7	143.5(7)
O(21)-W(5)-O(99)#5	157.6(7)	O(98)#6-K(1)-C(7)#7	105.4(7)
O(9)-W(5)-O(99)#5	93.9(8)	O(2)#9-K(1)-C(7)#7	79.3(6)
O(15)-W(5)-O(99)#5	64.1(6)	C(11)#7-K(1)-C(7)#7	27.7(7)
O(16)-W(5)-O(99)#5	92.5(7)	N(4)-K(1)-N(6)	22.8(5)
O(8)-W(5)-O(99)#5	60.4(8)	C(8)#3-K(1)-N(6)	99.0(6)
O(21)-W(5)-O(1)	157.9(6)	C(12)#3-K(1)-N(6)	90.1(7)
O(9)-W(5)-O(1)	60.0(8)	O(98)#6-K(1)-N(6)	153.2(5)
O(15)-W(5)-O(1)	92.4(5)	O(2)#9-K(1)-N(6)	94.6(5)
O(16)-W(5)-O(1)	66.0(7)	C(11)#7-K(1)-N(6)	83.7(7)
O(8)-W(5)-O(1)	94.5(8)	C(7)#7-K(1)-N(6)	74.0(6)
O(99)#5-W(5)-O(1)	44.4(6)	N(4)-K(1)-O(14)#6	80.3(5)
C(11)#7-K(1)-O(18)#6	66.1(7)	O(2)#9-K(1)-O(18)#6	69.6(5)
C(8)#3-K(1)-O(18)#6	118.6(6)	N(6)-K(1)-O(18)#6	139.8(5)
N(4)-K(1)-C(8)#3	87.0(7)	O(14)#6-K(1)-O(18)#6	105.2(4)
N(4)-K(1)-C(12)#3	88.6(8)	N(4)-K(1)-N(2)	16.9(5)
C(8)#3-K(1)-C(12)#3	28.5(7)	C(8)#3-K(1)-N(2)	89.0(6)
C(12)#3-K(1)-N(2)	98.2(7)	O(18)#6-K(1)-Ag(3)#3	114.9(3)
O(98)#6-K(1)-N(2)	116.7(5)	C(8)#3-K(1)-Ag(3)#3	99.9(5)
O(2)#9-K(1)-N(2)	131.6(6)	C(12)#3-K(1)-Ag(3)#3	76.1(6)
C(11)#7-K(1)-N(2)	81.0(7)	O(98)#6-K(1)-Ag(3)#3	166.9(4)
C(7)#7-K(1)-N(2)	88.8(6)	O(2)#9-K(1)-Ag(3)#3	55.5(4)
O(14)#6-K(1)-N(2)	66.0(4)	C(7)#7-K(1)-Ag(3)#3	70.9(5)
O(18)#6-K(1)-N(2)	145.7(5)	N(6)-K(1)-Ag(3)#3	39.1(3)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+3/2,z+1/2; #2 x-1,y,z; #3 x+1,-y+3/2,z+1/2; #4 x-1,-y+3/2,z+1/2; #5 -x,-y+2,-z+2; #6 x,-y+3/2,z-1/2; #7 x+1,y,z; #8 x-1,-y+3/2,z-1/2; #9 x+1,-y+3/2, z-1/2.