Electronic Supplementary Material (ESI) for CrystEngComm.

Rigid organic ligand induced POMCPs with helical self-penetrating structure as redox- and acid-catalyst

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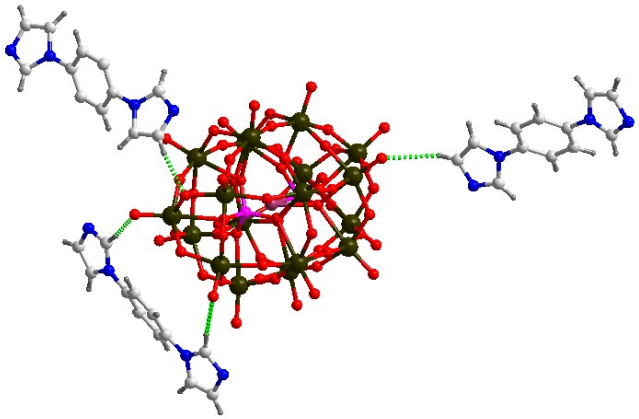

Figure S1. Combined ball and stick representation of the asymmetric unit of compound 2. Water molecules and all hydrogen atoms are omitted for clarity.

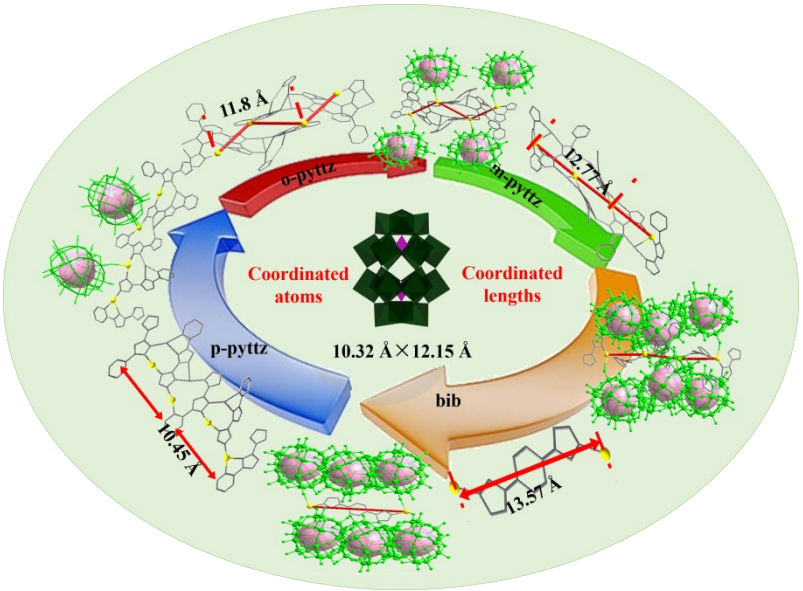

Figure S2. The influence of the coordinated lengths of organic ligands (pyttz and bib) on the structures of helix.

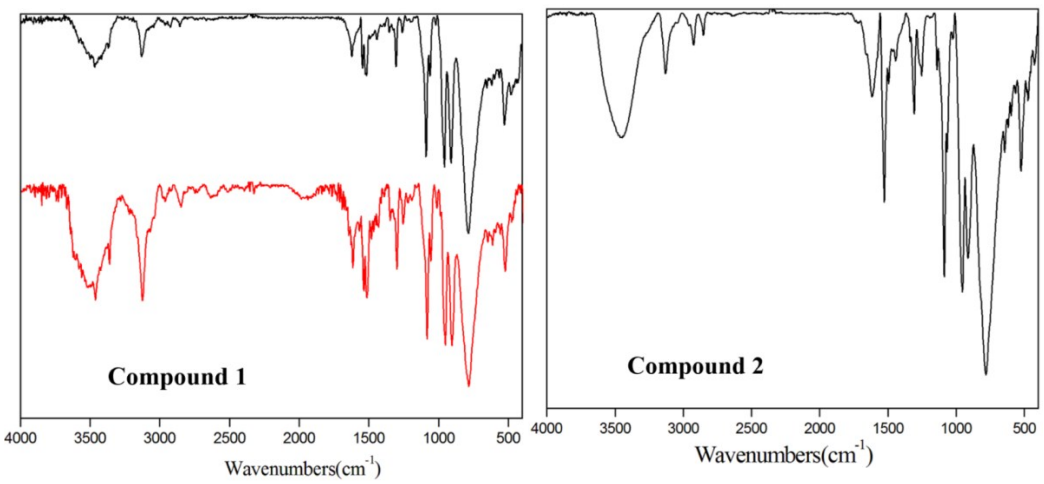

Figure S3. The IR spectra of the compounds **1** before (black) and after (red) the catalytic experiment and compound **2**.

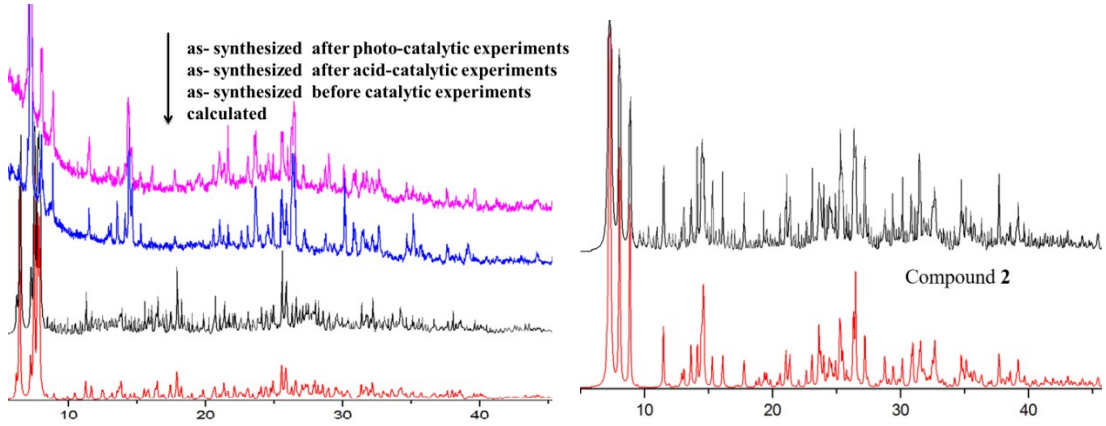

Figure S4. The simulated (below) and experimental (top) XRD pattern of compounds **1** and **2**.

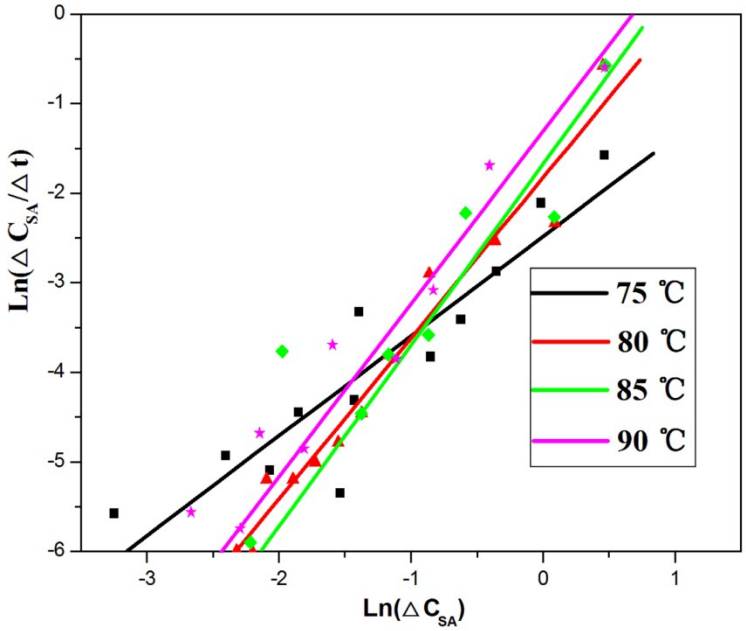

Figure S5. The linear relation of ln ($\Delta C_{SA}/\Delta t$) with ln C_{SA} at 75°C, 80°C, 85°C and 90°C.

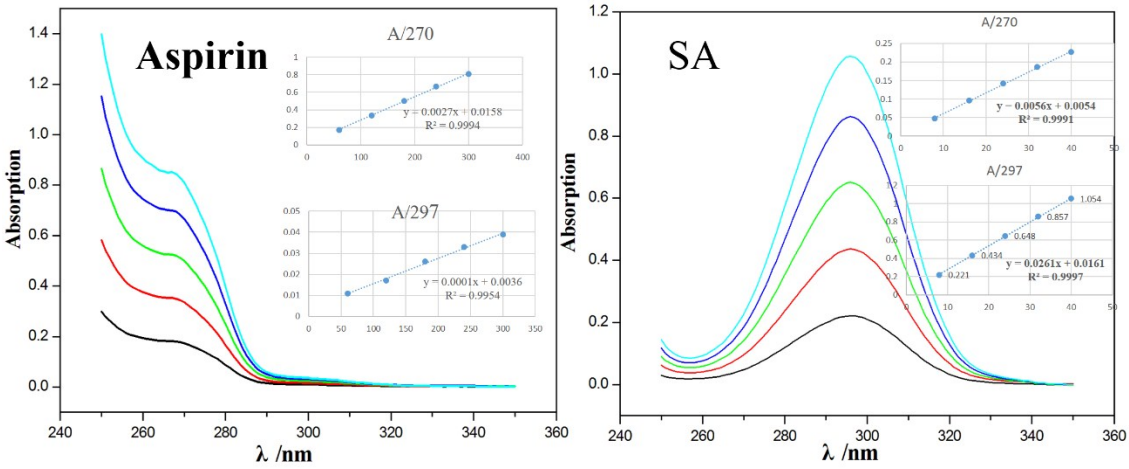

Figure S6 The UV and standard curve of Aspirin and SA.

ESI† The establishment of the detection method of ultraviolet two-wavelength isoabsorption spectrophotometry.

The standard curve equation

The precision amount of SA standard was dissolved in 0.002M phosphate buffer solution, then making into a certain mass concentration as the reference substance solution: 8ug.ml^{-1}, 16ug.ml^{-1}, 24ug.ml^{-1}, 32ug.ml^{-1} and 40ug.ml^{-1}; According to the same method, the Aspirin reference substance solution, 60ug.ml^{-1}, 120ug.ml^{-1}, 180ug.ml^{-1}, 240ug.ml^{-1} and 300ug.ml^{-1}, are obtained. According to the UV spectrophotometry of SA, ASP and their mixture, the measure wavelength is determined to be 270nm and 297nm in Figure S6. The process of standard curve equation is as follows:

$A_{270}=A_{ASP270}+A_{SA270}$

$A_{297}=A_{ASP297}+A_{SA297}$

$A_{ASP270} = 0.0027C_{ASP} + 0.0158$ ($R^2 = 0.9994$) (1)

$A_{ASP297} = 0.0001C_{ASP} + 0.0036$ ($R^2 = 0.9954$) (2)

$A_{SA270} = 0.0056C_{SA} + 0.0054$ ($R^2 = 0.9991$) (3)

$A_{SA297} = 0.0261C_{SA} + 0.0161$ ($R^2 = 0.9997$) (4)

The final equation can be worked out by equations 1, 2, 3 and 4.

$$C_{SA} = 38.6211A_{297} - 1.4304A_{270} - 0.7297 \quad (5)$$

$$C_{ASP} = 372.0272A_{270} - 80.12827A_{297} + 6.3389 \quad (6)$$

Table S1. Comparison of salicylic acid conversion, yield of ASP, Conversion of SA and catalytic selectivity catalyzed by compound **1**.

Catalyst (30 mg)	T/℃	t(min)											
		5	10	15	20	25	30	35	40	45	50	55	60
Yield (%)	75	34.77	53.03	68.03	74.06	79.43	83.08	86.22	87.66	89.11	89.56	89.70	89.93
	80	39.25	57.16	72.99	77.20	82.64	88.48	89.80	90.35	90.01	89.66	88.78	88.58
	85	43.64	63.49	78.26	85.37	89.39	90.34	93.79	92.89	91.69	90.16	89.71	89.13
	90	50.30	70.78	82.88	86.82	90.93	93.77	92.73	90.36	89.37	88.14	87.96	87.11
Conversion (%)	75	63.41	68.39	79.92	87.73	90.23	92.34	94.56	95.11	96.14	96.64	96.86	97.12
	80	66.59	73.84	83.97	90.31	92.16	93.20	95.17	95.94	96.57	97.21	97.49	97.78
	85	70.98	77.39	87.18	91.15	92.90	94.21	96.23	96.96	97.21	97.52	97.65	97.78
	90	76.14	84.63	89.97	92.46	95.34	96.25	97.33	97.70	97.92	97.98	98.43	98.58
Selectivity (%)	75	54.83	77.54	85.12	86.42	88.03	89.97	91.18	92.17	92.69	92.67	92.61	92.60
	80	58.94	77.41	86.92	88.48	89.67	92.94	94.35	94.17	93.21	92.23	91.07	90.59
	85	61.48	82.04	89.77	93.66	96.22	95.89	97.46	95.80	94.32	92.45	91.87	91.15
	90	66.06	83.64	92.12	93.90	95.37	97.42	95.27	92.49	91.27	89.96	89.36	88.37

Table S2. Concentration and conversation of SA at 75°C

t(min)	C_{SA}(mol/L)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.590916	63.40905	0.46431	-1.57658
10	0.984905	68.39252	-0.01521	-2.1103
15	0.702036	79.91778	-0.35377	-2.87221
20	0.536864	87.72622	-0.62201	-3.41021
25	0.428078	90.23293	-0.84845	-3.82783
30	0.248605	92.33927	-1.39189	-3.32716
35	0.239536	94.5568	-1.42905	-4.31226
40	0.215799	95.10612	-1.53341	-5.35018
45	0.157132	96.14381	-1.85067	-4.44531
50	0.12645	96.644	-2.06791	-5.09354
55	0.090327	96.86403	-2.40432	-4.93026
60	0.038915	97.12465	-3.24638	-5.57732

Table S3. Concentration and conversation of SA at 80 °C

t(min)	C_{SA}(mol/L)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.582981	66.59142	0.45931	-0.57376

10	1.097319	73.84434	0.09287	-2.33167
15	0.699549	83.97477	-0.35732	-2.53132
20	0.423725	90.31276	-0.85867	-2.89744
25	0.312819	92.16275	-1.16213	-3.80849
30	0.254565	93.20356	-1.3682	-4.4524
35	0.212586	95.16921	-1.54841	-4.78001
40	0.179106	95.93824	-1.71978	-5.00625
45	0.151379	96.574	-1.88797	-5.19478
50	0.123651	97.20721	-2.09029	-5.19478
55	0.111316	97.49092	-2.19538	-6.00478
60	0.098826	97.777	-2.31439	-5.99225

Table S4. Concentration and conversation of SA at 85 °C

t(min)	C_{SA}(mol/L)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.609768	70.97516	0.47609	-0.58332
10	1.095915	77.39252	0.09159	-2.27524
15	0.559563	87.18151	-0.5806	-2.2324
20	0.421911	91.15423	-0.86296	-3.59247
25	0.311315	92.89704	-1.16695	-3.81129
30	0.25415	94.213	-1.36983	-4.47126
35	0.13951	96.22977	-1.96962	-3.77539
40	0.134115	96.95854	-2.00906	-6.83169
45	0.123237	97.21091	-2.09365	-6.13042
50	0.109658	97.52326	-2.21039	-5.9087
55	0.104165	97.65213	-2.26178	-6.81361
60	0.098702	97.7798	-2.31565	-6.81928

Table S5. Concentration and conversation of SA at 90 °C

t(min)	C_{SA}(mol/L)	Conversion (%)	Ln C_{SA}	Ln($\Delta C_{SA}/\Delta t$)
5	1.602476	76.14323	0.47155	-0.5807
10	0.66959	84.6302	-0.40109	-1.67892
15	0.437771	89.97153	-0.82606	-3.07123
20	0.329971	92.45617	-1.10875	-3.83692
25	0.204087	95.34357	-1.58921	-3.68181
30	0.164542	96.25337	-1.80459	-4.83979
35	0.117536	97.32912	-2.14101	-4.6669
40	0.101366	97.70122	-2.28902	-5.73404
45	0.09183	97.92171	-2.38782	-6.26211
50	0.089291	97.98329	-2.41586	-7.58523

55	0.069855	98.42546	-2.66133	-5.55012
60	0.063066	98.58139	-2.76357	-6.60185

Table S6. Reaction rate constants under various temperatures of compound **1**.

T/K	348	353	358	363
1/T	0.002874	0.002833	0.002793	0.002755
Ln K	-2.4827	-1.83	-1.6934	-1.0806

Table S7. Selected bond lengths and angles of Compound **1**

Bond	**Lengths**	**Bond**	**Lengths**
Ag(4B)-O(58)#1	2.44(2)	O(13)-W(7)	1.93(2)
Ag(4B)-O(53)	2.54(2)	O(14)-W(8)	1.69(2)
Ag(4B)-O(48)	2.58(3)	O(15)-W(4)	1.702(19)
O(51)-W(16)	1.72(2)	O(16)-W(5)	1.906(19)
O(52)-W(8)	1.906(18)	O(16)-W(4)	1.909(19)
O(52)-W(6)	1.92(2)	O(17)-W(5)	1.70(2)
O(53)-W(11)#4	1.68(2)	O(18)-P(1)	1.520(19)
O(54)-W(18)	1.88(2)	O(18)-W(5)	2.335(17)
O(54)-W(11)	1.91(2)	O(18)-W(4)	2.389(16)
O(55)-W(18)	1.701(19)	O(19)-W(6)	1.85(2)
O(56)-W(7)	1.692(19)	O(19)-W(5)	1.928(19)
O(57)-W(15)	1.66(2)	O(20)-W(4)	1.889(17)
O(58)-W(14)	1.67(2)	O(20)-W(7)	1.897(18)
O(58)-Ag(4B)#1	2.44(2)	O(21)-W(12)	1.89(2)
O(59)-W(6)	1.691(19)	O(21)-W(5)	1.90(2)
O(60)-W(3)	1.68(2)	O(22)-W(4)	1.82(2)
O(61)-W(9)	1.887(19)	O(22)-W(11)	1.98(2)
O(61)-W(8)	1.916(19)	O(24)-W(18)	1.87(2)
O(62)-P(2)	1.57(2)	O(24)-W(7)	1.92(2)
O(62)-W(16)	2.37(2)	O(25)-W(15)	1.86(2)
O(62)-W(13)	2.39(2)	O(25)-W(8)	1.95(2)
O(62)-W(17)	2.43(2)	O(26)-W(10)	1.88(2)
O(63)-W(9)	1.72(2)	O(26)-W(9)	1.91(2)
W(10)-O(01)	1.71(2)	O(27)-W(14)	1.87(2)
W(11)-O(53)#4	1.68(2)	O(27)-W(6)	1.92(2)
O(6)-W(3)	1.87(2)	O(28)-P(1)	1.524(18)

O(6)-W(5)	1.95(2)	O(28)-W(7)	2.344(18)
O(7)-W(2)	1.87(2)	O(28)-W(9)	2.345(19)
O(7)-W(4)	1.96(2)	O(29)-P(1)	1.537(19)
O(8)-W(3)	1.88(2)	O(29)-W(8)	2.347(19)
O(8)-W(6)	1.94(2)	O(29)-W(6)	2.362(17)
O(9)-P(1)	1.64(2)	O(30)-W(12)	1.71(2)
O(9)-W(2)	2.33(2)	O(31)-W(11)	1.907(18)
O(9)-W(3)	2.34(2)	O(31)-W(12)	1.928(19)
O(9)-W(1)	2.37(2)	O(32)-W(12)	1.89(2)
O(10)-W(7)	1.88(2)	O(32)-W(14)	1.90(2)
O(10)-W(2)	1.93(2)	O(33)-P(2)	1.55(2)
O(11)-W(8)	1.89(2)	O(33)-W(12)	2.331(18)
O(11)-W(1)	1.93(2)	O(33)-W(11)	2.354(19)
O(12)-W(1)	1.90(2)	O(34)-P(2)	1.510(19)
O(12)-W(9)	1.93(2)	O(34)-W(14)	2.352(17)
O(13)-W(9)	1.88(2)	O(34)-W(15)	2.371(18)
N(3)-Ag(1)	2.11(3)	O(35)-P(2)	1.502(19)
N(4)-Ag(2)	2.05(3)	O(35)-W(10)	2.363(19)
N(5)-Ag(2)	2.11(3)	O(35)-W(18)	2.377(18)
N(6)-Ag(1)	2.13(3)	O(36)-W(14)	1.877(18)
N(7)-Ag(3)	2.14(3)	O(36)-W(15)	1.936(17)
O(1)-W(1)	1.71(2)	O(37)-W(15)	1.892(17)
O(2)-W(3)	1.91(2)	O(37)-W(10)	1.894(18)
O(2)-W(1)	1.938(19)	O(38)-W(18)	1.888(18)
O(3)-W(1)	1.932(19)	O(38)-W(10)	1.908(17)
O(3)-W(2)	1.94(2)	O(39)-W(15)	1.90(2)
O(4)-W(2)	1.73(2)	O(39)-W(16)	1.924(19)
O(5)-W(2)	1.90(2)	O(40)-W(10)	1.87(2)
O(5)-W(3)	1.93(2)	O(40)-W(16)	1.94(2)
N(11)-Ag(3)	2.07(3)	O(41)-W(14)	1.89(3)
O(45)-W(11)	1.86(2)	O(41)-W(17)	1.93(2)
O(45)-W(13)	1.92(2)	O(42)-W(13)	1.89(2)
O(46)-W(13)	1.72(2)	O(42)-W(18)	1.94(2)
O(47)-W(17)	1.89(2)	O(44)-W(12)	1.87(2)
O(47)-W(13)	1.90(2)	O(44)-W(17)	1.91(2)
O(48)-W(17)	1.74(3)	O(50)-W(16)	1.89(2)
O(49)-W(16)	1.844(19)	O(50)-W(13)	1.90(2)
Bonds	**Angle**	**Bonds**	**Angles**

O(58)#1-Ag(4B)-O(53)	154.2(9)	O(19)-W(6)-O(8)	84.8(9)
O(58)#1-Ag(4B)-O(48)	86.3(9)	O(27)-W(6)-O(8)	163.8(8)
O(53)-Ag(4B)-O(48)	73.0(8)	O(52)-W(6)-O(8)	89.1(10)
O(51)-W(16)-O(39)	104.6(10)	O(59)-W(6)-O(29)	170.2(9)
O(18)-P(1)-O(28)	112.2(11)	O(19)-W(6)-O(29)	85.4(7)
O(28)-P(1)-O(29)	113.8(10)	O(27)-W(6)-O(29)	82.7(7)
O(18)-P(1)-O(9)	105.3(11)	O(52)-W(6)-O(29)	72.1(7)
O(28)-P(1)-O(9)	103.8(11)	O(8)-W(6)-O(29)	81.5(7)
O(29)-P(1)-O(9)	107.0(11)	O(56)-W(7)-O(10)	99.8(11)
O(35)-P(2)-O(34)	112.3(12)	O(56)-W(7)-O(20)	102.3(9)
O(35)-P(2)-O(33)	112.5(11)	O(10)-W(7)-O(20)	86.7(9)
O(34)-P(2)-O(33)	112.8(10)	O(56)-W(7)-O(24)	98.5(11)
O(35)-P(2)-O(62)	104.7(11)	O(10)-W(7)-O(24)	161.6(8)
O(34)-P(2)-O(62)	107.7(11)	O(20)-W(7)-O(24)	88.0(9)
O(33)-P(2)-O(62)	106.2(12)	O(56)-W(7)-O(13)	101.1(9)
N(3)-Ag(1)-N(6)	172.2(12)	O(10)-W(7)-O(13)	89.2(9)
N(4)-Ag(2)-N(5)	178.2(13)	O(20)-W(7)-O(13)	156.7(8)
N(11)-Ag(3)-N(7)	176.6(12)	O(24)-W(7)-O(13)	88.8(9)
O(1)-W(1)-O(12)	102.2(10)	O(56)-W(7)-O(28)	173.1(10)
O(15)-W(4)-O(18)	173.7(8)	O(10)-W(7)-O(28)	78.7(8)
O(22)-W(4)-O(18)	82.8(8)	O(20)-W(7)-O(28)	84.4(8)
O(20)-W(4)-O(18)	85.0(7)	O(24)-W(7)-O(28)	83.3(7)
O(16)-W(4)-O(18)	72.7(7)	O(13)-W(7)-O(28)	72.2(7)
O(7)-W(4)-O(18)	80.6(7)	O(14)-W(8)-O(11)	98.1(11)
O(17)-W(5)-O(21)	98.1(11)	O(14)-W(8)-O(52)	100.1(10)
O(17)-W(5)-O(16)	100.1(9)	O(11)-W(8)-O(52)	91.4(10)
O(21)-W(5)-O(16)	91.6(9)	O(14)-W(8)-O(61)	102.1(9)
O(17)-W(5)-O(19)	102.0(9)	O(11)-W(8)-O(61)	86.2(9)
O(21)-W(5)-O(19)	88.2(9)	O(52)-W(8)-O(61)	157.8(9)
O(16)-W(5)-O(19)	157.7(8)	O(14)-W(8)-O(25)	97.8(11)
O(17)-W(5)-O(6)	98.4(11)	O(11)-W(8)-O(25)	163.8(9)
O(21)-W(5)-O(6)	163.0(8)	O(52)-W(8)-O(25)	88.7(10)
O(16)-W(5)-O(6)	89.5(9)	O(61)-W(8)-O(25)	87.6(9)
O(19)-W(5)-O(6)	84.4(9)	O(14)-W(8)-O(29)	172.8(8)
O(17)-W(5)-O(18)	174.1(8)	O(11)-W(8)-O(29)	82.1(9)
O(21)-W(5)-O(18)	81.9(7)	O(52)-W(8)-O(29)	72.7(7)
O(16)-W(5)-O(18)	74.0(7)	O(61)-W(8)-O(29)	85.1(7)
O(19)-W(5)-O(18)	83.9(7)	O(25)-W(8)-O(29)	82.5(8)

O(6)-W(5)-O(18)	82.1(7)	O(63)-W(9)-O(13)	99.0(9)
O(59)-W(6)-O(19)	103.8(9)	O(63)-W(9)-O(61)	101.2(9)
O(59)-W(6)-O(27)	100.3(10)	O(13)-W(9)-O(61)	158.9(8)
O(19)-W(6)-O(27)	90.3(9)	O(63)-W(9)-O(26)	99.8(10)
O(59)-W(6)-O(52)	98.5(9)	O(13)-W(9)-O(26)	93.5(9)
O(19)-W(6)-O(52)	157.4(8)	O(61)-W(9)-O(26)	89.1(9)
O(27)-W(6)-O(52)	89.6(10)	O(63)-W(9)-O(12)	95.1(10)
O(59)-W(6)-O(8)	95.9(10)	O(13)-W(9)-O(12)	88.4(9)
O(22)-W(4)-O(16)	93.0(9)	O(61)-W(9)-O(12)	83.8(9)
O(20)-W(4)-O(16)	157.0(9)	O(26)-W(9)-O(12)	164.5(9)
O(15)-W(4)-O(7)	96.2(11)	O(63)-W(9)-O(28)	170.0(9)
O(22)-W(4)-O(7)	162.9(8)	O(13)-W(9)-O(28)	73.0(7)
O(20)-W(4)-O(7)	85.0(9)	O(61)-W(9)-O(28)	86.3(8)
O(11)-W(1)-O(2)	87.5(8)	O(26)-W(9)-O(28)	86.7(8)
O(1)-W(1)-O(9)	169.6(9)	O(12)-W(9)-O(28)	79.1(9)
O(12)-W(1)-O(9)	85.1(9)	O(01)-W(10)-O(40)	99.1(10)
O(3)-W(1)-O(9)	73.1(8)	O(01)-W(10)-O(26)	96.5(11)
O(11)-W(1)-O(9)	84.5(9)	O(40)-W(10)-O(26)	164.1(8)
O(2)-W(1)-O(9)	72.5(8)	O(01)-W(10)-O(37)	103.3(10)
O(4)-W(2)-O(7)	103.1(11)	O(40)-W(10)-O(37)	86.3(8)
O(4)-W(2)-O(5)	102.7(10)	O(26)-W(10)-O(37)	87.4(8)
O(7)-W(2)-O(5)	89.9(9)	O(01)-W(10)-O(38)	98.8(9)
O(4)-W(2)-O(10)	102.2(9)	O(40)-W(10)-O(38)	91.1(8)
O(7)-W(2)-O(10)	86.2(9)	O(26)-W(10)-O(38)	89.3(8)
O(5)-W(2)-O(10)	155.0(9)	O(37)-W(10)-O(38)	157.9(8)
O(4)-W(2)-O(3)	98.6(11)	O(01)-W(10)-O(35)	171.6(9)
O(7)-W(2)-O(3)	158.2(8)	O(40)-W(10)-O(35)	82.7(8)
O(5)-W(2)-O(3)	87.5(9)	O(26)-W(10)-O(35)	82.2(8)
O(10)-W(2)-O(3)	87.1(9)	O(37)-W(10)-O(35)	85.0(8)
O(4)-W(2)-O(9)	170.8(11)	O(38)-W(10)-O(35)	72.9(7)
O(7)-W(2)-O(9)	84.9(8)	O(53)#4-W(11)-O(45)	98.2(9)
O(5)-W(2)-O(9)	72.3(8)	O(53)#4-W(11)-O(31)	100.6(9)
O(10)-W(2)-O(9)	82.7(8)	O(45)-W(11)-O(31)	91.3(8)
O(3)-W(2)-O(9)	73.7(8)	O(53)#4-W(11)-O(54)	101.0(9)
O(60)-W(3)-O(6)	100.6(12)	O(45)-W(11)-O(54)	86.6(9)
O(60)-W(3)-O(8)	103.0(11)	O(31)-W(11)-O(54)	158.4(8)
O(6)-W(3)-O(8)	86.1(9)	O(53)#4-W(11)-O(22)	100.0(9)
O(60)-W(3)-O(2)	102.1(12)	O(45)-W(11)-O(22)	161.5(8)

O(6)-W(3)-O(2)	157.2(9)	O(31)-W(11)-O(22)	88.6(8)
O(8)-W(3)-O(2)	90.7(9)	O(54)-W(11)-O(22)	86.6(8)
O(60)-W(3)-O(5)	99.8(11)	O(53)#4-W(11)-O(33)	174.4(8)
O(6)-W(3)-O(5)	86.2(9)	O(45)-W(11)-O(33)	81.2(8)
O(8)-W(3)-O(5)	156.9(9)	O(31)-W(11)-O(33)	73.9(8)
O(2)-W(3)-O(5)	88.0(9)	O(54)-W(11)-O(33)	84.5(8)
O(60)-W(3)-O(9)	170.2(12)	O(22)-W(11)-O(33)	81.0(7)
O(6)-W(3)-O(9)	83.7(8)	O(30)-W(12)-O(44)	98.3(10)
O(8)-W(3)-O(9)	85.9(8)	O(30)-W(12)-O(32)	101.3(9)
O(2)-W(3)-O(9)	73.5(8)	O(44)-W(12)-O(32)	83.6(9)
O(5)-W(3)-O(9)	71.6(8)	O(30)-W(12)-O(21)	97.9(9)
O(15)-W(4)-O(22)	100.8(11)	O(44)-W(12)-O(21)	162.8(9)
O(15)-W(4)-O(20)	100.2(9)	O(32)-W(12)-O(21)	87.6(9)
O(22)-W(4)-O(20)	89.3(9)	O(30)-W(12)-O(31)	100.8(9)
O(15)-W(4)-O(16)	101.8(9)	O(44)-W(12)-O(31)	90.7(8)
O(1)-W(1)-O(3)	99.0(10)	O(32)-W(12)-O(31)	157.7(8)
O(12)-W(1)-O(3)	91.9(9)	O(21)-W(12)-O(31)	92.0(9)
O(1)-W(1)-O(11)	103.4(10)	O(30)-W(12)-O(33)	174.8(8)
O(12)-W(1)-O(11)	84.8(9)	O(44)-W(12)-O(33)	80.7(8)
O(3)-W(1)-O(11)	157.5(10)	O(32)-W(12)-O(33)	83.7(7)
O(1)-W(1)-O(2)	100.8(10)	O(21)-W(12)-O(33)	83.7(8)
O(12)-W(1)-O(2)	156.9(10)	O(31)-W(12)-O(33)	74.1(7)
O(3)-W(1)-O(2)	86.9(8)	O(46)-W(13)-O(42)	100.8(10)
O(49)-W(16)-O(39)	89.3(8)	O(46)-W(13)-O(50)	101.1(10)
O(50)-W(16)-O(39)	154.8(9)	O(42)-W(13)-O(50)	89.4(9)
O(51)-W(16)-O(40)	101.7(10)	O(46)-W(13)-O(47)	103.8(11)
O(49)-W(16)-O(40)	158.2(9)	O(42)-W(13)-O(47)	155.4(10)
O(50)-W(16)-O(40)	86.9(9)	O(50)-W(13)-O(47)	87.3(10)
O(39)-W(16)-O(40)	84.8(8)	O(46)-W(13)-O(45)	105.5(10)
O(51)-W(16)-O(62)	171.2(10)	O(42)-W(13)-O(45)	83.7(9)
O(49)-W(16)-O(62)	76.1(8)	O(50)-W(13)-O(45)	153.3(9)
O(50)-W(16)-O(62)	71.9(8)	O(47)-W(13)-O(45)	88.4(9)
O(39)-W(16)-O(62)	83.4(8)	O(46)-W(13)-O(62)	172.0(9)
O(40)-W(16)-O(62)	82.4(8)	O(42)-W(13)-O(62)	82.3(8)
O(48)-W(17)-O(47)	102.4(11)	O(50)-W(13)-O(62)	71.4(8)
O(48)-W(17)-O(44)	104.0(10)	O(47)-W(13)-O(62)	73.5(9)
O(47)-W(17)-O(44)	92.3(9)	O(45)-W(13)-O(62)	82.1(8)
O(48)-W(17)-O(41)	102.5(11)	O(58)-W(14)-O(27)	95.4(11)

O(47)-W(17)-O(41)	155.1(10)	O(58)-W(14)-O(36)	98.9(10)
O(44)-W(17)-O(41)	82.8(9)	O(27)-W(14)-O(36)	89.0(9)
O(48)-W(17)-O(49)	101.7(10)	O(58)-W(14)-O(41)	99.8(11)
O(47)-W(17)-O(49)	88.2(9)	O(27)-W(14)-O(41)	164.6(8)
O(44)-W(17)-O(49)	153.6(9)	O(36)-W(14)-O(41)	91.2(9)
O(41)-W(17)-O(49)	85.8(8)	O(58)-W(14)-O(32)	103.6(10)
O(48)-W(17)-O(62)	171.8(9)	O(27)-W(14)-O(32)	87.3(9)
O(47)-W(17)-O(62)	72.7(9)	O(36)-W(14)-O(32)	157.5(8)
O(44)-W(17)-O(62)	82.9(8)	O(41)-W(14)-O(32)	86.7(9)
O(41)-W(17)-O(62)	82.5(9)	O(58)-W(14)-O(34)	172.1(10)
O(49)-W(17)-O(62)	72.0(7)	O(27)-W(14)-O(34)	82.5(8)
O(55)-W(18)-O(24)	98.3(10)	O(36)-W(14)-O(34)	73.6(7)
O(55)-W(18)-O(54)	101.7(10)	O(41)-W(14)-O(34)	82.8(8)
O(24)-W(18)-O(54)	87.9(9)	O(32)-W(14)-O(34)	83.9(7)
O(55)-W(18)-O(38)	100.5(10)	O(57)-W(15)-O(25)	99.9(11)
O(24)-W(18)-O(38)	91.8(8)	O(57)-W(15)-O(37)	102.7(10)
O(54)-W(18)-O(38)	157.6(8)	O(25)-W(15)-O(37)	90.1(9)
O(55)-W(18)-O(42)	97.9(10)	O(57)-W(15)-O(39)	97.1(10)
O(24)-W(18)-O(42)	163.4(7)	O(25)-W(15)-O(39)	162.9(8)
O(54)-W(18)-O(42)	85.8(9)	O(37)-W(15)-O(39)	85.2(8)
O(38)-W(18)-O(42)	88.3(9)	O(57)-W(15)-O(36)	100.0(9)
O(55)-W(18)-O(35)	173.2(10)	O(25)-W(15)-O(36)	89.8(8)
O(24)-W(18)-O(35)	83.7(7)	O(37)-W(15)-O(36)	157.0(8)
O(54)-W(18)-O(35)	84.7(7)	O(39)-W(15)-O(36)	88.2(8)
O(38)-W(18)-O(35)	72.9(7)	O(57)-W(15)-O(34)	171.8(10)
O(42)-W(18)-O(35)	80.5(7)	O(25)-W(15)-O(34)	82.7(8)
O(51)-W(16)-O(49)	100.1(11)	O(37)-W(15)-O(34)	85.0(7)
O(51)-W(16)-O(50)	100.4(11)	O(39)-W(15)-O(34)	80.6(7)
O(49)-W(16)-O(50)	89.7(9)	O(36)-W(15)-O(34)	72.2(7)

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

Table S8. Selected bond lengths and angles of Compound **2**

Bond	**Lengths**	**Bond**	**Lengths**
O(1)-P(1)	1.518(9)	O(18)-W(6)	1.898(9)
O(1)-W(6)	2.357(9)	O(19)-W(2)	1.908(9)
O(1)-W(9)	2.393(9)	O(19)-W(7)	1.927(10)

O(2)-W(2)	1.708(9)	O(20)-W(4)	1.899(9)
O(3)-P(1)	1.518(9)	O(20)-W(1)	1.964(9)
O(3)-W(3)	2.356(8)	O(21)-W(5)	1.716(9)
O(3)-W(5)	2.376(8)	O(22)-W(2)	1.900(9)
O(4)-P(1)	1.587(10)	O(22)-W(4)	1.933(8)
O(4)-W(1)	2.361(9)	O(23)-W(6)#1	1.893(10)
O(4)-W(4)	2.369(9)	O(23)-W(3)	1.902(10)
O(4)-W(2)	2.380(9)	O(24)-W(3)	1.712(10)
O(5)-W(4)	1.910(10)	O(25)-W(1)	1.899(9)
O(5)-W(8)	1.915(10)	O(25)-W(2)	1.933(10)
O(6)-W(1)	1.882(10)	O(26)-W(7)	1.911(9)
O(6)-W(5)	1.944(10)	O(26)-W(8)	1.913(9)
O(7)-W(8)	1.697(9)	O(27)-W(1)	1.709(10)
O(8)-W(3)	1.895(10)	O(32)-P(1)	1.539(9)
O(8)-W(2)	1.920(10)	O(32)-W(8)	2.350(9)
O(9)-W(7)	1.877(9)	O(32)-W(7)	2.359(8)
O(9)-W(3)	1.911(9)	O(28)-W(7)	1.715(9)
O(11)-W(1)	1.901(9)	O(29)-W(6)	1.700(9)
O(11)-W(9)	1.910(10)	O(30)-W(4)	1.695(9)
O(12)-W(4)	1.894(9)	O(31)-W(9)	1.715(10)
O(12)-W(6)	1.942(10)	W(6)-O(23)#1	1.893(10)
O(13)-W(5)	1.877(10)	W(7)-O(17)#1	1.891(10)
O(13)-W(9)#1	1.907(10)	W(9)-O(13)#1	1.907(10)
O(14)-W(9)	1.889(10)	O(15)-W(9)	1.915(9)
O(14)-W(6)	1.918(10)	O(16)-W(3)	1.898(9)
O(15)-W(5)	1.869(9)	O(16)-W(5)	1.919(9)
O(17)-W(8)	1.909(10)	O(17)-W(7)#1	1.891(10)
Bond	**angles**	**Bond**	**angles**
O(3)-P(1)-O(1)	112.7(5)	O(15)-W(5)-O(3)	84.6(4)
O(3)-P(1)-O(32)	111.6(5)	O(13)-W(5)-O(3)	83.5(3)
O(1)-P(1)-O(32)	111.7(5)	O(16)-W(5)-O(3)	72.8(3)
O(3)-P(1)-O(4)	106.6(5)	O(6)-W(5)-O(3)	81.1(4)
O(1)-P(1)-O(4)	107.2(5)	O(29)-W(6)-O(23)#1	99.4(5)
O(32)-P(1)-O(4)	106.6(5)	O(29)-W(6)-O(18)	101.6(4)
O(27)-W(1)-O(6)	101.9(5)	O(23)#1-W(6)-O(18)	89.4(4)
O(27)-W(1)-O(25)	100.8(5)	O(29)-W(6)-O(14)	100.9(4)
O(6)-W(1)-O(25)	91.6(4)	O(23)#1-W(6)-O(14)	90.5(4)
O(27)-W(1)-O(11)	101.9(5)	O(18)-W(6)-O(14)	157.2(4)
O(6)-W(1)-O(11)	85.9(4)	O(29)-W(6)-O(12)	96.7(5)
O(25)-W(1)-O(11)	157.3(4)	O(23)#1-W(6)-O(12)	163.8(4)
O(27)-W(1)-O(20)	100.8(4)	O(18)-W(6)-O(12)	85.8(4)
O(6)-W(1)-O(20)	157.1(4)	O(14)-W(6)-O(12)	88.0(4)
O(25)-W(1)-O(20)	87.4(4)	O(29)-W(6)-O(1)	174.1(4)
O(11)-W(1)-O(20)	86.3(4)	O(23)#1-W(6)-O(1)	83.4(4)

O(27)-W(1)-O(4)	171.2(4)	O(18)-W(6)-O(1)	83.6(3)
O(6)-W(1)-O(4)	84.9(4)	O(14)-W(6)-O(1)	73.7(3)
O(25)-W(1)-O(4)	73.3(4)	O(12)-W(6)-O(1)	80.8(4)
O(11)-W(1)-O(4)	84.0(4)	O(28)-W(7)-O(9)	102.9(4)
O(20)-W(1)-O(4)	72.9(4)	O(28)-W(7)-O(17)#1	99.3(5)
O(2)-W(2)-O(22)	103.4(4)	O(9)-W(7)-O(17)#1	90.1(4)
O(2)-W(2)-O(19)	103.4(5)	O(28)-W(7)-O(26)	100.4(4)
O(22)-W(2)-O(19)	89.4(4)	O(9)-W(7)-O(26)	156.4(4)
O(2)-W(2)-O(8)	101.1(5)	O(17)#1-W(7)-O(26)	89.8(4)
O(22)-W(2)-O(8)	155.5(4)	O(28)-W(7)-O(19)	96.6(5)
O(19)-W(2)-O(8)	85.8(4)	O(9)-W(7)-O(19)	86.1(4)
O(2)-W(2)-O(25)	99.9(5)	O(17)#1-W(7)-O(19)	164.1(4)
O(22)-W(2)-O(25)	86.9(4)	O(26)-W(7)-O(19)	87.7(4)
O(19)-W(2)-O(25)	156.6(4)	O(28)-W(7)-O(32)	172.9(4)
O(8)-W(2)-O(25)	88.1(4)	O(9)-W(7)-O(32)	83.8(3)
O(2)-W(2)-O(4)	171.5(4)	O(17)#1-W(7)-O(32)	82.7(4)
O(22)-W(2)-O(4)	73.2(3)	O(26)-W(7)-O(32)	72.7(3)
O(19)-W(2)-O(4)	84.5(3)	O(19)-W(7)-O(32)	81.6(4)
O(8)-W(2)-O(4)	82.4(4)	O(7)-W(8)-O(18)	101.6(4)
O(25)-W(2)-O(4)	72.3(3)	O(7)-W(8)-O(17)	99.4(5)
O(24)-W(3)-O(8)	97.6(5)	O(18)-W(8)-O(17)	88.0(4)
O(24)-W(3)-O(16)	99.8(4)	O(7)-W(8)-O(26)	100.7(4)
O(8)-W(3)-O(16)	91.1(4)	O(18)-W(8)-O(26)	157.6(4)
O(24)-W(3)-O(23)	97.8(5)	O(17)-W(8)-O(26)	90.8(4)
O(8)-W(3)-O(23)	164.0(4)	O(7)-W(8)-O(5)	96.7(5)
O(16)-W(3)-O(23)	90.2(4)	O(18)-W(8)-O(5)	86.1(4)
O(24)-W(3)-O(9)	103.0(4)	O(17)-W(8)-O(5)	163.7(4)
O(8)-W(3)-O(9)	85.2(4)	O(26)-W(8)-O(5)	88.9(4)
O(16)-W(3)-O(9)	157.2(4)	O(7)-W(8)-O(32)	173.2(4)
O(23)-W(3)-O(9)	87.4(4)	O(18)-W(8)-O(32)	84.7(3)
O(24)-W(3)-O(3)	173.4(4)	O(17)-W(8)-O(32)	83.2(4)
O(8)-W(3)-O(3)	82.2(4)	O(26)-W(8)-O(32)	72.9(3)
O(16)-W(3)-O(3)	73.6(3)	O(5)-W(8)-O(32)	81.0(4)
O(23)-W(3)-O(3)	82.9(4)	O(31)-W(9)-O(14)	99.6(5)
O(9)-W(3)-O(3)	83.6(3)	O(31)-W(9)-O(13)#1	99.4(5)
O(30)-W(4)-O(12)	101.7(4)	O(14)-W(9)-O(13)#1	90.2(4)
O(30)-W(4)-O(20)	101.5(4)	O(31)-W(9)-O(11)	97.5(5)
O(12)-W(4)-O(20)	88.7(4)	O(14)-W(9)-O(11)	91.6(4)
O(30)-W(4)-O(5)	101.4(4)	O(13)#1-W(9)-O(11)	162.5(4)
O(12)-W(4)-O(5)	86.4(4)	O(31)-W(9)-O(15)	103.5(5)
O(20)-W(4)-O(5)	157.1(4)	O(14)-W(9)-O(15)	156.9(4)
O(30)-W(4)-O(22)	100.5(4)	O(13)#1-W(9)-O(15)	86.2(4)
O(12)-W(4)-O(22)	157.7(4)	O(11)-W(9)-O(15)	85.2(4)
O(20)-W(4)-O(22)	88.4(4)	O(31)-W(9)-O(1)	172.9(4)

O(5)-W(4)-O(22)	87.8(4)	O(14)-W(9)-O(1)	73.3(4)
O(30)-W(4)-O(4)	171.8(4)	O(13)#1-W(9)-O(1)	82.1(4)
O(12)-W(4)-O(4)	85.0(4)	O(11)-W(9)-O(1)	81.8(4)
O(20)-W(4)-O(4)	73.8(4)	O(15)-W(9)-O(1)	83.5(4)
O(5)-W(4)-O(4)	83.5(4)	O(21)-W(5)-O(16)	99.9(4)
O(22)-W(4)-O(4)	73.0(3)	O(15)-W(5)-O(16)	157.0(4)
O(21)-W(5)-O(15)	102.6(5)	O(13)-W(5)-O(16)	90.2(4)
O(21)-W(5)-O(13)	98.1(4)	O(21)-W(5)-O(6)	97.5(5)
O(15)-W(5)-O(13)	91.0(4)	O(15)-W(5)-O(6)	85.4(4)
O(16)-W(5)-O(6)	87.3(4)	O(13)-W(5)-O(6)	164.4(4)

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