

Supporting Information

Captions

- Table S1.** Bond lengths [\AA] and angles [$^\circ$] for compound **1**
Figure S1. SEM images of bipyramid-shaped single crystals for **1**
Figure S2. Energy dispersive spectroscopy for **1**
Figure S3. Simulated and experimental powder X-ray diffraction patterns of **1**
Figure S4. TG curve of compound **1**
Figure S5. IR spectrum of compound **1**

Table S1. Bond lengths [Å] and angles [°] for compound **1**

Bond lengths [Å]			
B(1)-O(3)#1	1.460(8)	P(1)-O(3)	1.530(8)
B(1)-O(3)#2	1.460(8)	Ti(1)-O(2)#5	1.914(6)
B(1)-O(3)	1.460(8)	Ti(1)-O(2)	1.914(6)
B(1)-O(3)#3	1.460(8)	Ti(1)-O(1)#6	1.935(4)
P(1)-O(2)	1.502(6)	Ti(1)-O(1)#7	1.935(4)
P(1)-O(1)	1.526(4)	Ti(1)-O(1)#8	1.935(4)
P(1)-O(1)#4	1.526(4)	Ti(1)-O(1)#9	1.935(4)
Bond angles [°]			
O(3)#1-B(1)-O(3)#2	112.6(3)	O(2)#5-Ti(1)-O(1)#7	90.19(12)
O(3)#1-B(1)-O(3)	112.6(3)	O(2)-Ti(1)-O(1)#7	89.81(12)
O(3)#2-B(1)-O(3)	103.4(6)	O(1)#6-Ti(1)-O(1)#7	179.6(2)
O(3)#1-B(1)-O(3)#3	103.4(6)	O(2)#5-Ti(1)-O(1)#8	89.81(12)
O(3)#2-B(1)-O(3)#3	112.6(3)	O(2)-Ti(1)-O(1)#8	90.19(12)
O(3)-B(1)-O(3)#3	112.6(3)	O(1)#6-Ti(1)-O(1)#8	90.001(1)
O(2)-P(1)-O(1)	111.98(19)	O(1)#7-Ti(1)-O(1)#8	90.001(1)
O(2)-P(1)-O(1)#4	111.98(19)	O(2)#5-Ti(1)-O(1)#9	89.81(12)
O(1)-P(1)-O(1)#4	106.6(3)	O(2)-Ti(1)-O(1)#9	90.19(12)
O(2)-P(1)-O(3)	104.2(3)	O(1)#6-Ti(1)-O(1)#9	90.001(1)
O(1)-P(1)-O(3)	111.1(2)	O(1)#7-Ti(1)-O(1)#9	90.001(1)
O(1)#4-P(1)-O(3)	111.1(2)	O(1)#8-Ti(1)-O(1)#9	179.6(2)
O(2)#5-Ti(1)-O(2)	180.000(1)	P(1)-O(1)-Ti(1)#6	143.4(2)
O(2)#5-Ti(1)-O(1)#6	90.19(12)	P(1)-O(2)-Ti(1)	161.05(13)
O(2)-Ti(1)-O(1)#6	89.81(12)	B(1)-O(3)-P(1)	136.9(6)

Symmetry transformations used to generate equivalent atoms:

#1: -y+5/4, x-3/4, -z-1/4; #2: -x+2, -y+1/2, z; #3: y+3/4, -x+5/4, -z-1/4; #4: -x+1, -y+1/2, z;
 #5: y+1/4, -x+3/4, -z+1/4; #6: -x+1, -y, -z; #7: x, y+1/2, -z; #8: -y+1/4, x-1/4, z+1/4;
 #9: y+3/4, -x+3/4, z+1/4.

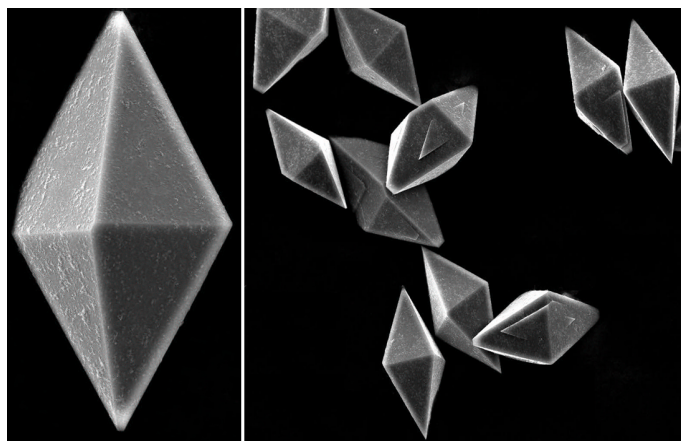


Figure S1. SEM images of bipyramid-shaped single crystals for **1**.

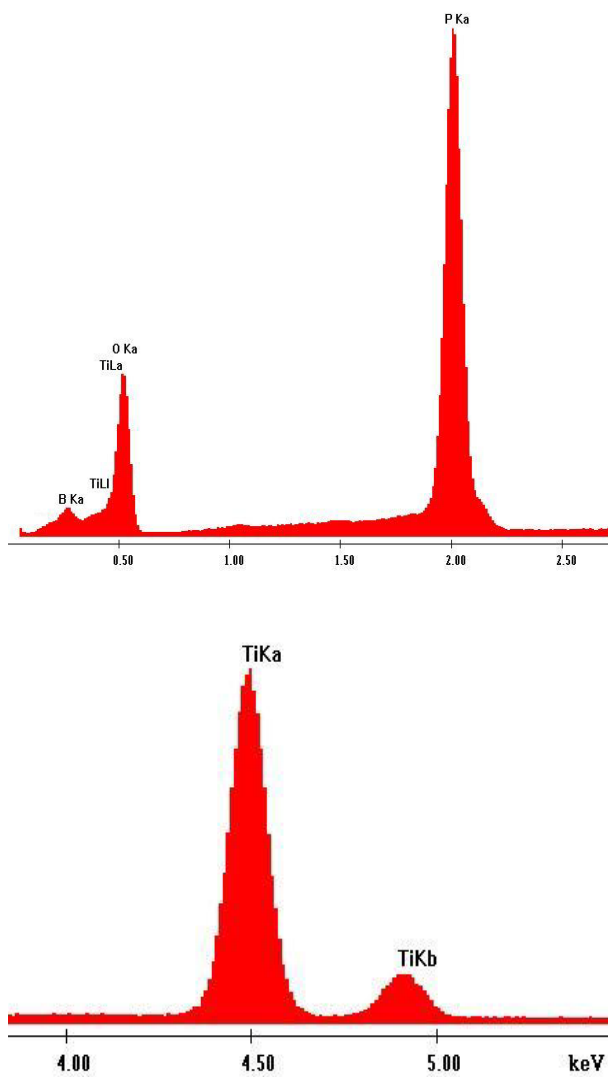


Figure S2. Energy dispersive spectroscopy for **1**

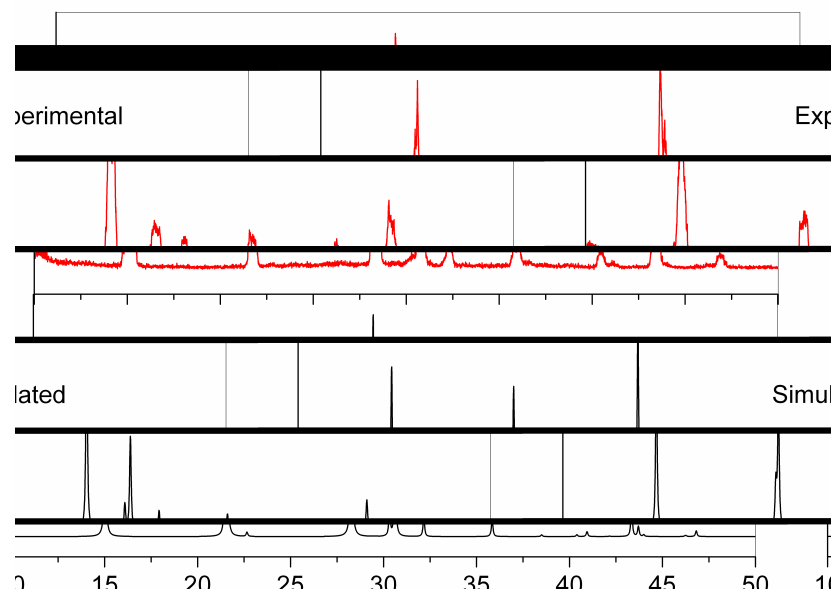


Figure S3. Simulated and experimental powder X-ray diffraction patterns of **1**

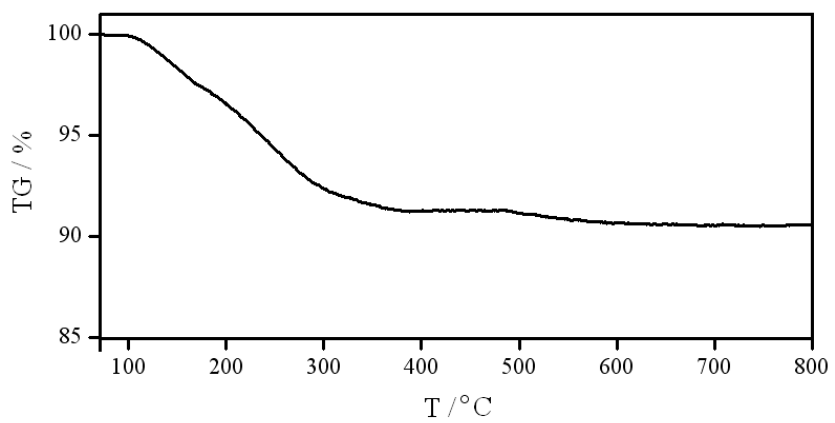


Figure S4. TG curve of compound 1

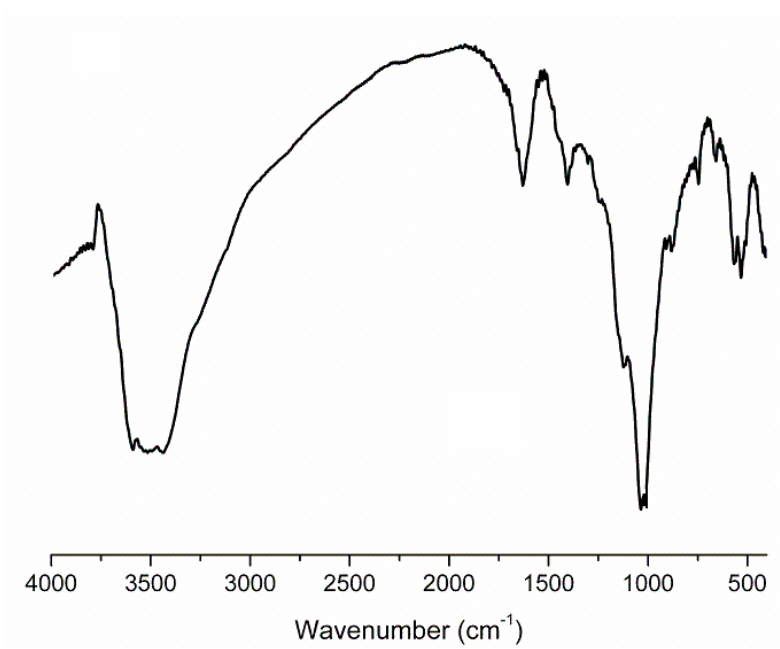


Figure S5. IR spectrum of compound **1**