Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Solvothermal syntheses and structures of four indium-phosphite coordination polymers

Xuelei Wang, Yan Yan, Junbiao Wu, Chuanqi Zhang, Jiyang Li*

Table S1a The bond lengths [Å] and bond angles [°] for InHPO-CJ11.

In(1)-O(1)#1	2.1335(15)	O(3)#7-In(2)-O(3)#8	91.04(6)
In(1)-O(1)#2	2.1336(15)	O(3)#6-In(2)-O(2)	91.56(5)
In(1)-O(1)#3	2.1336(15)	O(3)#7-In(2)-O(2)	177.33(5)
In(1)-O(1)#4	2.1336(15)	O(3)#8-In(2)-O(2)	89.53(5)
In(1)-O(1)	2.1336(15)	O(3)#6-In(2)-O(2)#9	177.33(5)
In(1)-O(1)#5	2.1336(15)	O(3)#7-In(2)-O(2)#9	89.53(5)
In(2)-O(3)#6	2.1341(14)	O(3)#8-In(2)-O(2)#9	91.56(5)
In(2)-O(3)#7	2.1342(14)	O(2)-In(2)-O(2)#9	87.84(5)
In(2)-O(3)#8	2.1342(14)	O(3)#6-In(2)-O(2)#10	89.53(5)
In(2)-O(2)	2.1416(13)	O(3)#7-In(2)-O(2)#10	91.56(5)
In(2)-O(2)#9	2.1416(13)	O(3)#8-In(2)-O(2)#10	177.32(5)
In(2)-O(2)#10	2.1417(13)	O(2)-In(2)-O(2)#10	87.84(5)
P(1)-P(1')	0.810(6)	O(2)#9-In(2)-O(2)#10	87.84(5)
P(1)-O(1)	1.5021(16)	P(1')-P(1)-O(1)	73.1(3)
P(1)-O(2)	1.5277(15)	P(1')-P(1)-O(2)	73.4(3)
P(1)-O(3)	1.5307(15)	O(1)-P(1)-O(2)	109.94(9)
P(1)-H(1P)	1.399(2)	P(1')-P(1)-O(3)	70.7(3)
P(1')-O(3)	1.476(4)	O(1)-P(1)-O(3)	112.80(10)
P(1')-O(1)	1.485(4)	O(2)-P(1)-O(3)	111.03(9)
P(1')-O(2)	1.511(4)	P(1')-P(1)-H(1P)	178.8(9)
O(3)-In(2)#8	2.1342(14)	O(1)-P(1)-H(1P)	105.9(9)
O(1)#1-In(1)-O(1)#2	93.65(6)	O(2)-P(1)-H(1P)	106.5(9)
O(1)#1-In(1)-O(1)#3	93.65(6)	O(3)-P(1)-H(1P)	110.4(9)
O(1)#2-In(1)-O(1)#3	93.65(6)	P(1)-P(1')-O(3)	78.2(3)
O(1)#1-In(1)-O(1)#4	86.35(6)	P(1)-P(1')-O(1)	75.4(4)
O(1)#2-In(1)-O(1)#4	180.00(6)	O(3)-P(1')-O(1)	117.1(3)
O(1)#3-In(1)-O(1)#4	86.35(6)	P(1)-P(1')-O(2)	75.7(3)
O(1)#1-In(1)-O(1)	86.35(6)	O(3)-P(1')-O(2)	115.1(3)
O(1)#2-In(1)-O(1)	86.35(6)	O(1)-P(1')-O(2)	111.8(3)
O(1)#3-In(1)-O(1)	180.0	P(1')-O(1)-P(1)	31.5(2)
O(1)#4-In(1)-O(1)	93.65(6)	P(1')-O(1)-In(1)	151.08(18)
O(1)#1-In(1)-O(1)#5	180.0	P(1)-O(1)-In(1)	137.95(11)
O(1)#2-In(1)-O(1)#5	86.35(6)	P(1')-O(2)-P(1)	30.9(2)
O(1)#3-In(1)-O(1)#5	86.35(6)	P(1')-O(2)-In(2)	143.98(18)
O(1)#4-In(1)-O(1)#5	93.65(6)	P(1)-O(2)-In(2)	124.67(8)
O(1)-In(1)-O(1)#5	93.65(6)	P(1')-O(3)-P(1)	31.2(2)
O(3)#6-In(2)-O(3)#7	91.04(6)	P(1')-O(3)-In(2)#8	155.4(2)
O(3)#6-In(2)-O(3)#8	91.04(6)	P(1)-O(3)-In(2)#8	129.78(9)

Symmetry transformations used to generate equivalent atoms: #1 y,-x+y,-z; #2 x-y,x,-z; #3 -x,-y,-z; #4 -x+y,-x,z; #5 -y,x-y,z; #6 y+2/3,-x+y+1/3,-z+1/3; #7 x-y+2/3,x+1/3,-z+1/3; #8 -x+2/3,-y+1/3,-z+1/3; #9 -x+y+1,-x+1,z; #10 -y+1,x-y,z.

Table S1b The bond lengths [Å] and bond angles [°] for InHPO-CJ12.

In(1)-O(4)#1	2.074(3)	O(5)#2-In(1)-O(6)	91.17(10
In(1)-O(5)#2	2.116(2)	O(3)-In(1)-O(6)	175.16(10)
In(1)-O(3)	2.122(3)	F(1)-In(1)-O(6)	88.23(10)
In(1)-F(1)	2.127(2)	O(4)#1-In(1)-O(2)	96.81(11)
In(1)-O(6)	2.138(3)	O(5)#2-In(1)-O(2)	162.36(9)
In(1)-O(2)	2.156(2)	O(3)-In(1)-O(2)	90.46(10)
P(1)-O(4)	1.485(3)	F(1)-In(1)-O(2)	80.49(8)
P(1)-O(5)	1.514(2)	O(6)-In(1)-O(2)	87.84(10)
P(1)-O(3)	1.520(3)	O(4)-P(1)-O(5)	112.70(16)
P(1)-H(1P)	1.3118	O(4)-P(1)-O(3)	114.28(17)
P(2)-O(1)	1.492(3)	O(5)-P(1)-O(3)	111.84(15)
P(2)-O(6)#3	1.529(3)	O(5)-P(1)-H(1P)	107.7
P(2)-O(2)	1.534(2)	O(3)-P(1)-H(1P)	107.7
P(2)-H(2P)	1.3999	O(1)-P(2)-O(6)#3	110.98(17)
O(4)-In(1)#1	2.074(3)	O(1)-P(2)-O(2)	111.03(17)
O(5)-In(1)#3	2.116(2)	O(6)#3-P(2)-O(2)	110.91(16)
O(6)-P(2)#2	1.529(3)	O(1)-P(2)-H(2P)	100.7
N(1)-C(1)	1.476(5)	O(6)#3-P(2)-H(2P)	109.6
N(2)-C(2)	1.502(5)	O(2)-P(2)-H(2P)	113.2
C(1)-C(2)	1.512(6)	P(2)-O(2)-In(1)	136.12(15)
C(2)-C(3)	1.517(5)	P(1)-O(3)-In(1)	133.01(16)
O(4)#1-In(1)-O(5)#2	100.82(11)	P(1)-O(4)-In(1)#1	172.7(2)
O(4)#1-In(1)-O(3)	92.90(12)	P(1)-O(5)-In(1)#3	140.55(16)
O(5)#2-In(1)-O(3)	89.08(10)	P(2)#2-O(6)-In(1)	131.73(15)
O(4)#1-In(1)-F(1)	177.30(10)	N(1)-C(1)-C(2)	114.4(3)
O(5)#2-In(1)-F(1)	81.88(9)	N(2)-C(2)-C(1)	111.1(3)
O(3)-In(1)-F(1)	87.02(9)	N(2)-C(2)-C(3)	108.3(4)
O(4)#1-In(1)-O(6)	91.79(13)	C(1)-C(2)-C(3)	110.1(4)

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

Table S1c. The bond lengths [Å] and bond angles [°] for InHPO-CJ13.

In(1)-O(1)	2.0680(17)	O(2)#3-In(1)-O(2)#4	73.60(7)
In(1)-O(1)#1	2.0680(17)	O(1)-In(1)-O(2)#5	90.18(8)
In(1)-O(1)#2	2.0680(17)	O(1)#1-In(1)-O(2)#5	161.78(7)
In(1)-O(2)#3	2.2082(16)	O(1)#2-In(1)-O(2)#5	94.18(7)
In(1)-O(2)#4	2.2082(16)	O(2)#3-In(1)-O(2)#5	73.60(7)
In(1)-O(2)#5	2.2082(16)	O(2)#4-In(1)-O(2)#5	73.60(7)
In(1)-In(1)#6	3.1894(5)	O(1)-In(1)-In(1)#6	118.26(5)
P(1)-O(1)#7	1.5059(18)	O(1)#1-In(1)-In(1)#6	118.26(5)
P(1)-O(1)	1.5059(18)	O(1)#2-In(1)-In(1)#6	118.26(5)
P(1)-O(2)	1.544(2)	O(2)#3-In(1)-In(1)#6	43.77(4)
P(1)-H(1P)	1.3027	O(2)#4-In(1)-In(1)#6	43.77(4)
O(2)-In(1)#4	2.2082(16)	O(2)#5-In(1)-In(1)#6	43.77(4)
O(2)-In(1)#8	2.2082(16)	O(1)#7-P(1)-O(1)	115.38(15)
O(1)-In(1)-O(1)#1	99.42(7)	O(1)#7-P(1)-O(2)	110.74(9)
O(1)-In(1)-O(1)#2	99.42(7)	O(1)-P(1)-O(2)	110.74(9)
O(1)#1-In(1)-O(1)#2	99.42(7)	O(1)#7-P(1)-H(1P)	105.0
O(1)-In(1)-O(2)#3	161.78(7)	O(1)-P(1)-H(1P)	105.0
O(1)#1-In(1)-O(2)#3	94.18(7)	O(2)-P(1)-H(1P)	109.6
O(1)#2-In(1)-O(2)#3	90.18(8)	P(1)-O(1)-In(1)	142.72(12)
O(1)-In(1)-O(2)#4	94.18(8)	P(1)-O(2)-In(1)#4	131.25(6)
O(1)#1-In(1)-O(2)#4	90.18(8)	P(1)-O(2)-In(1)#8	131.25(6)
O(1)#2-In(1)-O(2)#4	161.78(7)	In(1)#4-O(2)-In(1)#8	92.47(9)

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

Table S1d. The bond lengths [Å] and bond angles [°] for InHPO-CJ14.

In(1)-O(4)	2.1237(18)	O(5)#6-In(2)-O(5)#8	92.33(7)
In(1)-O(4)#1	2.1237(18)	O(5)#4-In(2)-O(5)#8	180.0
In(1)-O(4)#2	2.1237(18)	O(5)#7-In(2)-O(5)#8	92.33(7)
In(1)-O(4)#3	2.1237(18)	O(5)-In(2)-O(5)#8	87.67(7)
In(1)-O(4)#4	2.1237(18)	O(5)#4-In(2)-O(5)#5	92.33(7)
In(1)-O(4)#5	2.1237(18)	O(5)#7-In(2)-O(5)#5	87.67(7)
In(2)-O(5)#6	2.1402(16)	O(5)-In(2)-O(5)#5	92.33(7)
In(2)-O(5)#4	2.1402(16)	O(5)#8-In(2)-O(5)#5	87.67(7)
In(2)-O(5)#7	2.1403(16)	O(3)-In(3)-O(7)#9	97.10(8)
In(2)-O(5)	2.1403(16)	O(3)-In(3)-O(8)#6	87.91(9)
In(2)-O(5)#8	2.1403(16)	O(7)#9-In(3)-O(8)#6	93.17(7)
In(2)-O(5)#5	2.1403(16)	O(3)-In(3)-O(6)	91.85(8)
In(3)-O(3)	2.101(2)	O(7)#9-In(3)-O(6)	169.50(8)
In(3)-O(7)#9	2.102(2)	O(8)#6-In(3)-O(6)	92.63(9)
In(3)-O(8)#6	2.1137(16)	O(3)-In(3)-O(1)	94.96(9)
In(3)-O(6)	2.1164(18)	O(7)#9-In(3)-O(1)	90.07(7)
In(3)-O(1)	2.123(2)	O(8)#6-In(3)-O(1)	175.38(8)
In(3)-O(2)	2.2376(19)	O(6)-In(3)-O(1)	83.67(8)
P(1)-O(7)	1.4980(19)	O(3)-In(3)-O(2)	178.27(7)
P(1)-O(8)	1.5071(19)	O(7)#9-In(3)-O(2)	84.51(8)
P(1)-O(1)	1.516(2)	O(8)#6-In(3)-O(2)	92.66(8)
P(1)-H(1P)	1.4501(14)	O(6)-In(3)-O(2)	86.49(7)
P(2)-O(5)	1.520(2)	O(1)-In(3)-O(2)	84.37(8)
P(2)-O(4)	1.5218(19)	O(7)-P(1)-O(8)	111.98(13)
P(2)-O(6)	1.513(2)	O(7)-P(1)-O(1)	113.31(12)
P(2)-H(2P)	1.4503(13)	O(8)-P(1)-O(1)	110.53(10)
P(3)-O(3)#10	1.503(2)	O(7)-P(1)-H(1P)	103.55(13)
P(3)-O(3)#9	1.503(2)	O(8)-P(1)-H(1P)	109.72(10)
P(3)-O(3)	1.503(2)	O(1)-P(1)-H(1P)	107.39(14)
P(3)-H(3P)	1.4506(11)	O(5)-P(2)-O(4)	115.19(9)
P(3')-O(3)#10	1.441(2)	O(5)-P(2)-O(6)	112.79(12)
P(3')-O(3)#9	1.441(2)	O(4)-P(2)-O(6)	107.78(13)
P(3')-O(3)	1.441(2)	O(5)-P(2)-H(2P)	102.95(14)
O(7)-In(3)#10	2.102(2)	O(4)-P(2)-H(2P)	111.12(13)
O(8)-In(3)#8	2.1137(16)	O(6)-P(2)-H(2P)	106.67(12)
O(4)-In(1)-O(4)#1	176.62(12	O(3)#10-P(3)-O(3)#9	112.17(8)
O(4)-In(1)-O(4)#2	91.93(10)	O(3)#10-P(3)-O(3)	112.16(8)
O(4)#1-In(1)-O(4)#2	90.51(7)	O(3)#9-P(3)-O(3)	112.16(8)
O(4)-In(1)-O(4)#3	87.14(12)	O(3)#10-P(3)-H(3P)	106.62(9)
O(4)#1-In(1)-O(4)#3	90.51(7)	O(3)#9-P(3)-H(3P)	106.62(9)
O(4)#2-In(1)-O(4)#3	90.51(7)	O(3)-P(3)-H(3P)	106.62(9)
O(4)-In(1)-O(4)#4	90.52(7)	O(3)#10-P(3')-O(3)#9	119.96(3)

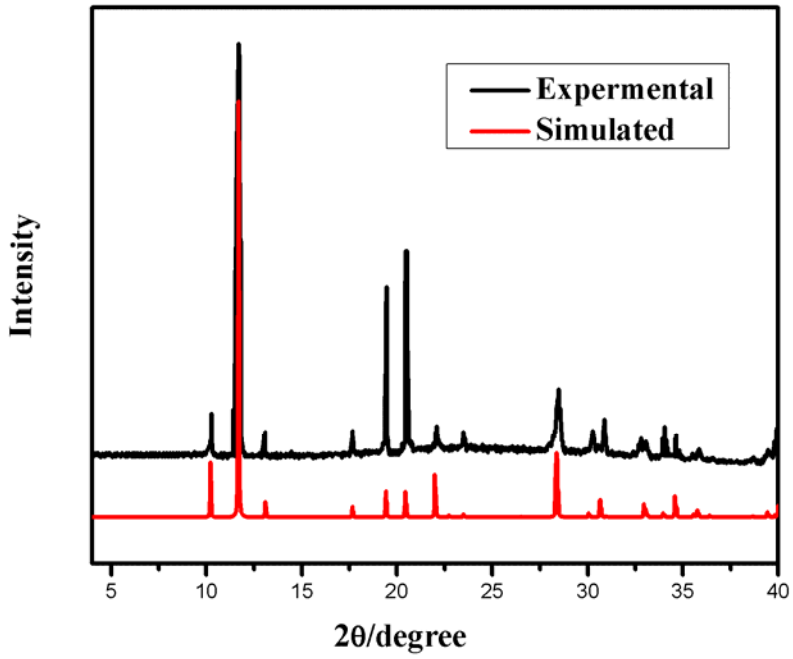
O(4)#1-In(1)-O(4)#4	91.93(10)	O(3)#10-P(3')-O(3)	119.95(3)
O(4)#2-In(1)-O(4)#4	87.14(12)	O(3)#9-P(3')-O(3)	119.95(3)
O(4)#3-In(1)-O(4)#4	176.62(12)	O(3)#10-P(3')-H(3P)	91.2(3)
O(4)-In(1)-O(4)#5	90.52(7)	O(3)#9-P(3')-H(3P)	91.2(3)
O(4)#1-In(1)-O(4)#5	87.14(12)	O(3)-P(3')-H(3P)	91.2(3)
O(4)#2-In(1)-O(4)#5	176.62(12)	P(1)-O(1)-In(3)	132.16(10)
O(4)#3-In(1)-O(4)#5	91.93(10)	P(3')-O(3)-P(3)	15.4(3)
O(4)#4-In(1)-O(4)#5	90.52(7)	P(3')-O(3)-In(3)	134.9(3)
O(5)#6-In(2)-O(5)#4	87.67(7)	P(3)-O(3)-In(3)	149.93(15)
O(5)#6-In(2)-O(5)#7	92.33(7)	P(2)-O(4)-In(1)	132.45(14)
O(5)#4-In(2)-O(5)#7	87.67(7)	P(2)-O(5)-In(2)	138.01(12)
O(5)#6-In(2)-O(5)	87.67(7)	P(2)-O(6)-In(3)	137.61(15)
O(5)#4-In(2)-O(5)	92.33(7)	P(1)-O(7)-In(3)#10	135.95(12)
O(5)#7-In(2)-O(5)	180.0	P(1)-O(8)-In(3)#8	136.33(13)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-x+y+1,-z+1/2; #2 y,x,-z+1/2; #3 x-y+1,-y+2,-z+1/2; #4 -y+2,x-y+1,z; #5 -x+y+1,-x+2,z; #6 x-y+1,x,-z; #7 -x+2,-y+2,-z; #8 y,-x+y+1,-z; #9 -x+y,-x+1,z; #10 -y+1,x-y+1,z.

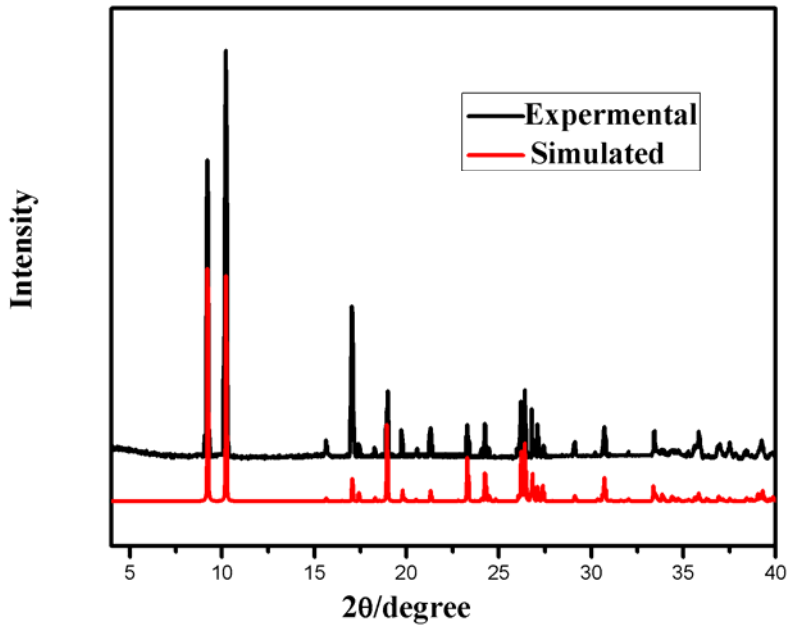
Table 2S. Hydrogen bonds for InHPO-CJ12 [Å and deg].

D-H⋯A	d(D-H)	d(H⋯A)	d(D⋯A)	<(DHA)
N(2)-H(2C)⋯O(1)#4	0.89	2.46	3.217(5)	142.9
N(2)-H(2C⋯O(6)#5	0.89	2.34	3.167(4)	153.9
N(2)-H(2B)⋯O(2)#6	0.89	2.04	2.920(4)	172.4
N(2)-H(2A)⋯O(1)#5	0.89	1.83	2.716(5)	173.2
N(1)-H(1C)⋯O(2)#6	0.89	2.03	2.918(4)	173.9
N(1)-H(1B)⋯O(5)#6	0.89	2.65	3.082(4)	110.9
N(1)-H(1B)⋯F(1)#7	0.89	1.93	2.735(4)	150.4
N(1)-H(1A)⋯F(1)#1	0.89	2.06	2.781(4)	137.5

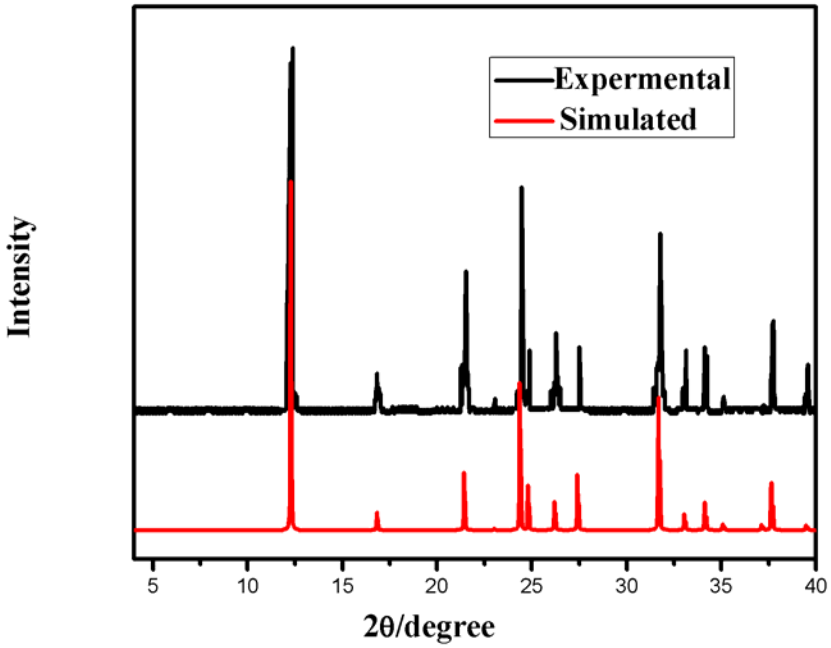
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1; #2 x+1,y,z; #3 x-1,y,z; #4 -x,-y+1,-z; #5 -x+1,-y+1,-z; #6 x,y+1,z; #7 x-1,y+1,z.



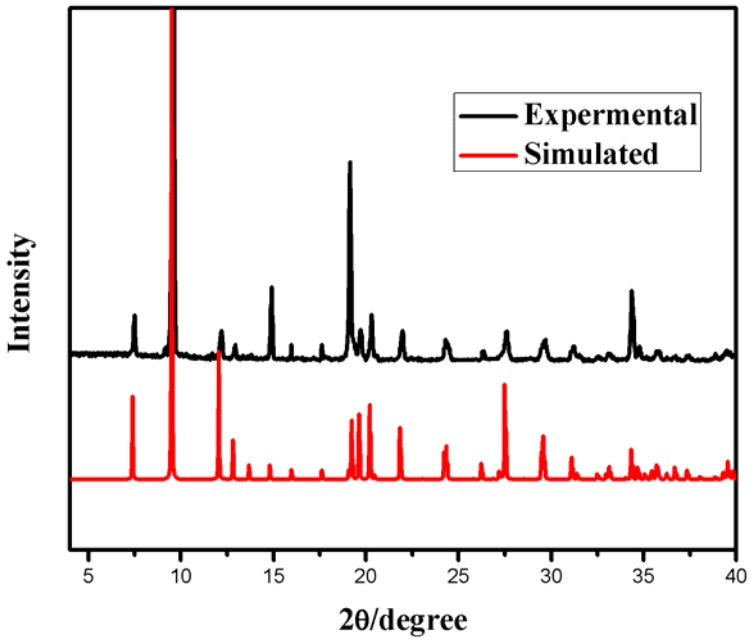
(a)



(b)

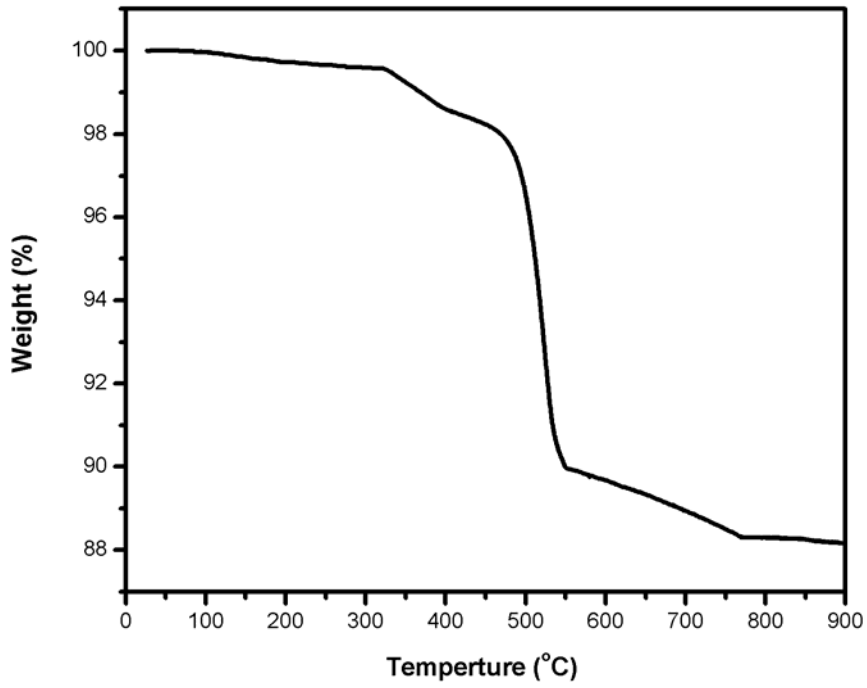


(c)

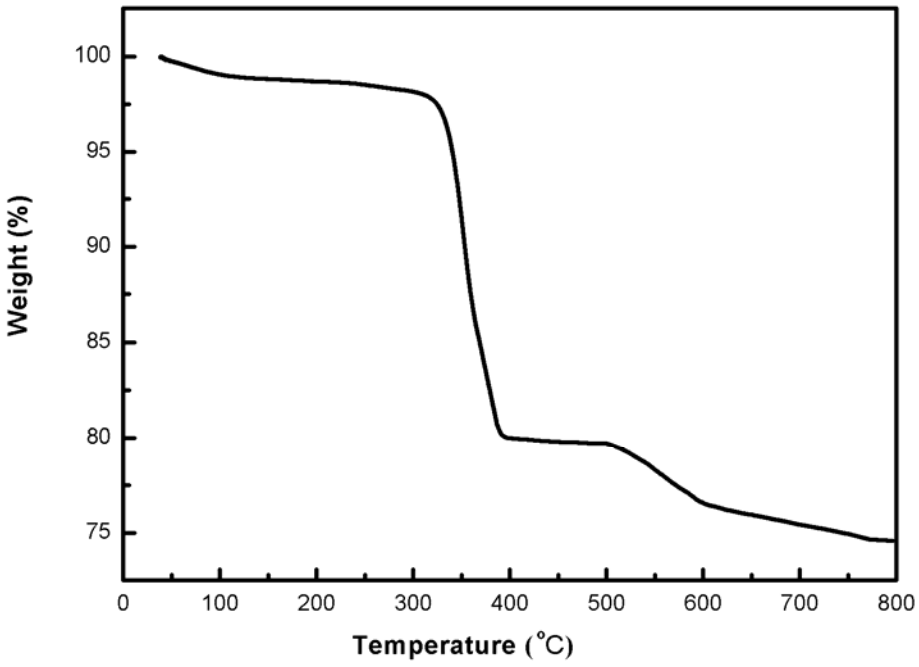


(d)

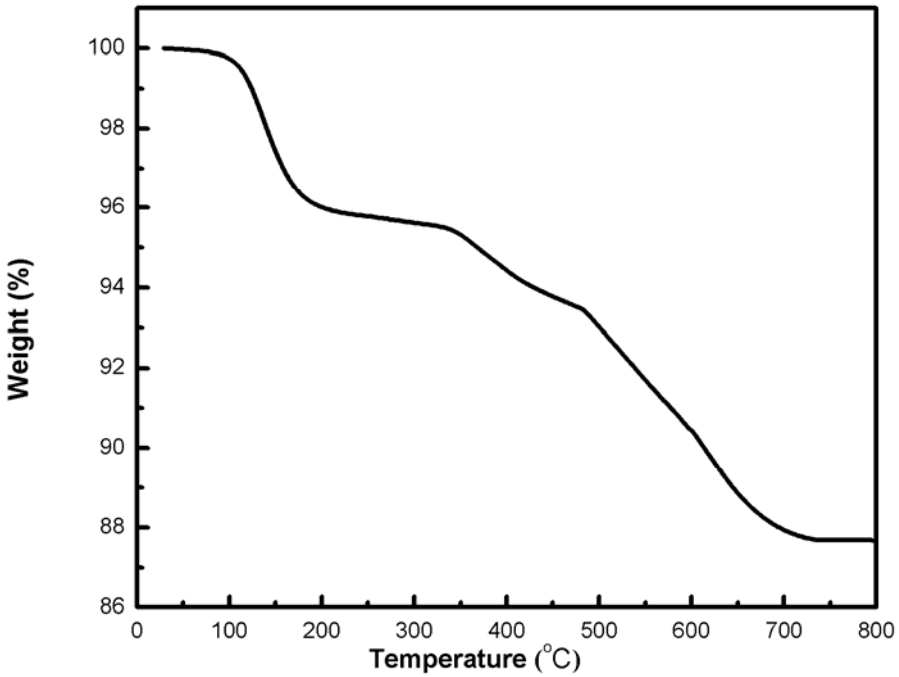
Figure S1. Experimental and simulated XRD patterns of (a) InHPO-CJ11, (b) InHPO-CJ12, (c) InHPO-CJ13 and (d) InHPO-CJ14.



(a)

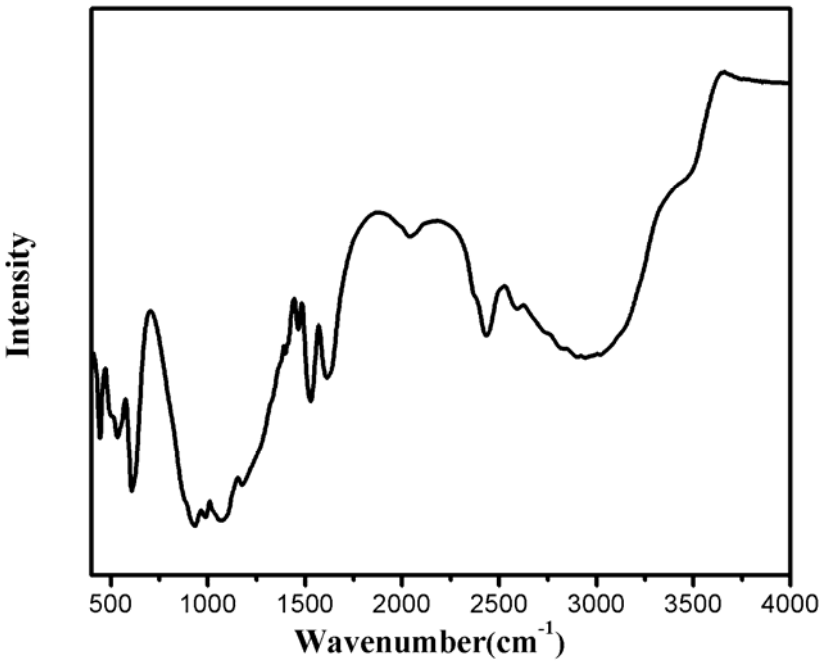


(b)

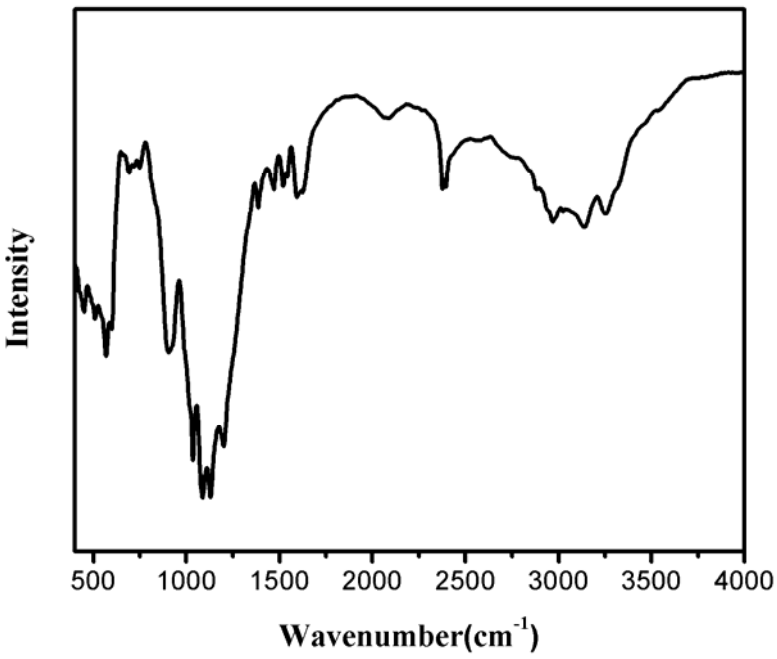


(c)

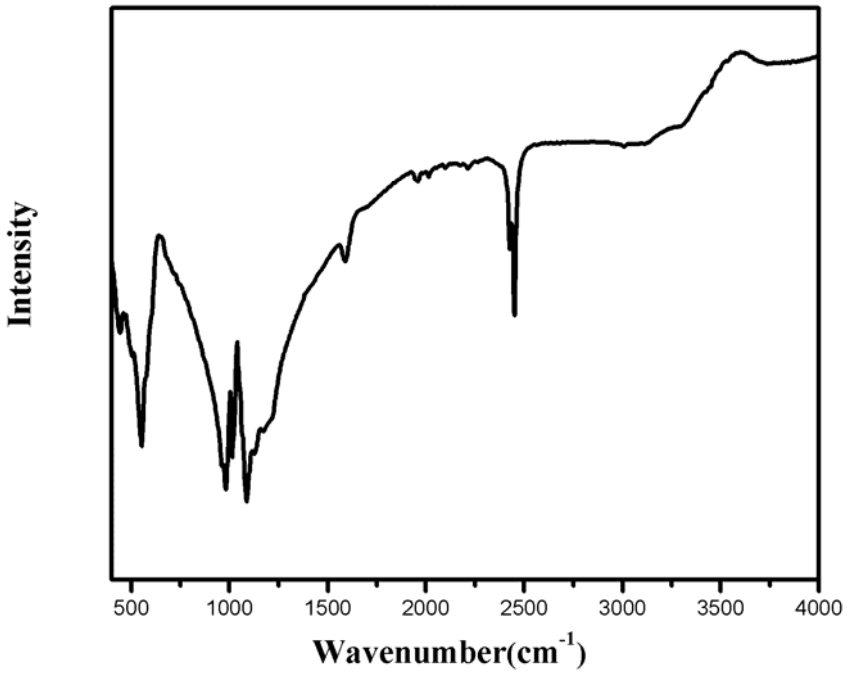
Figure S2. TG curves of (a) InHPO-CJ11, (b) InHPO-CJ12 and (c) InHPO-CJ14.



(a)



(b)



(c)

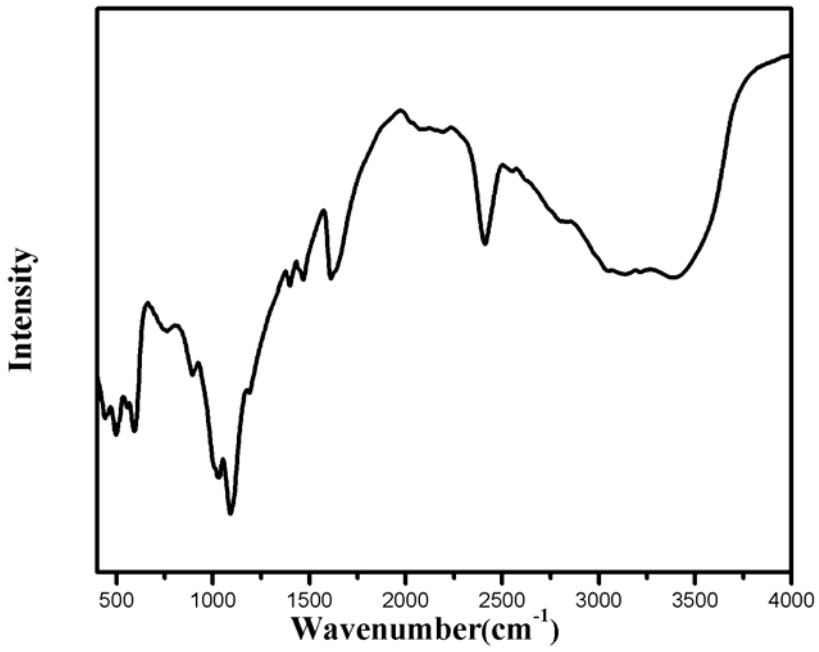
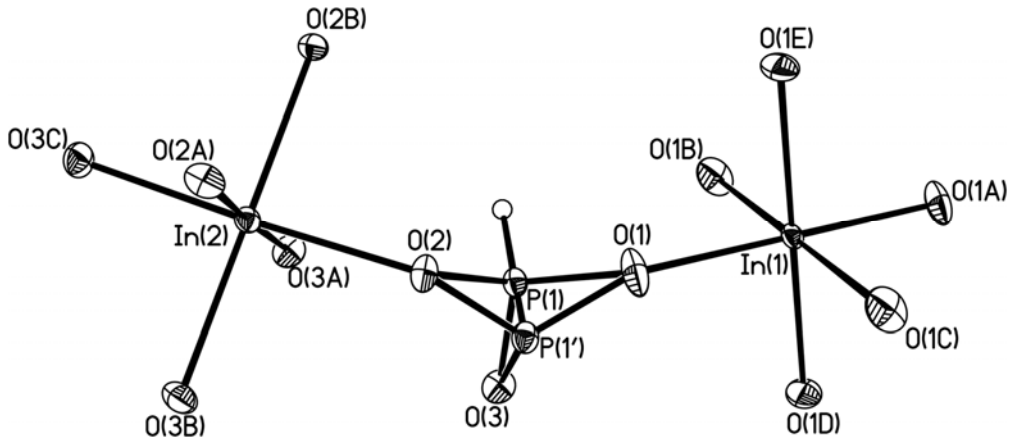
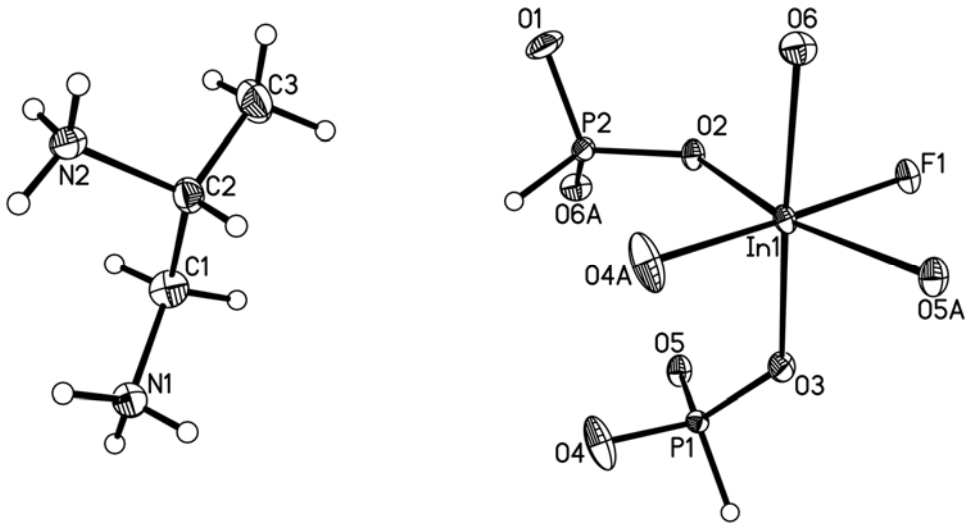


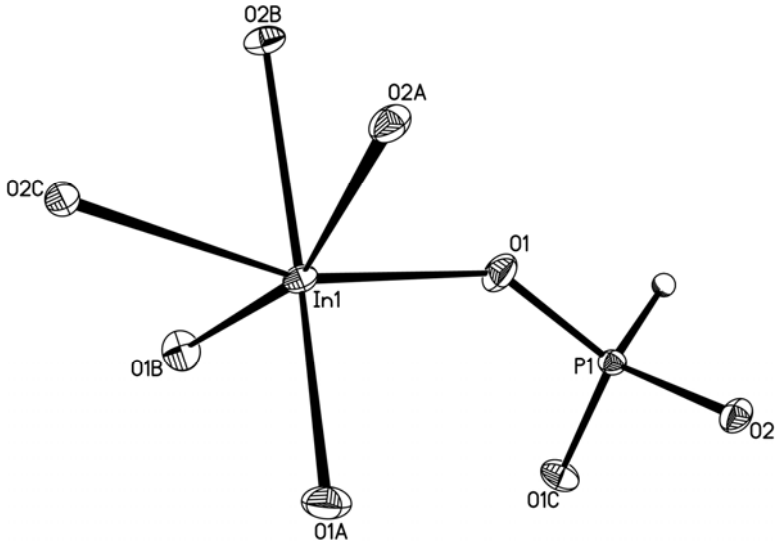
Figure S3. IR spectra of (a) InHPO-CJ11, (b) InHPO-CJ12, (c) InHPO-CJ13 and (d) InHPO-CJ14.



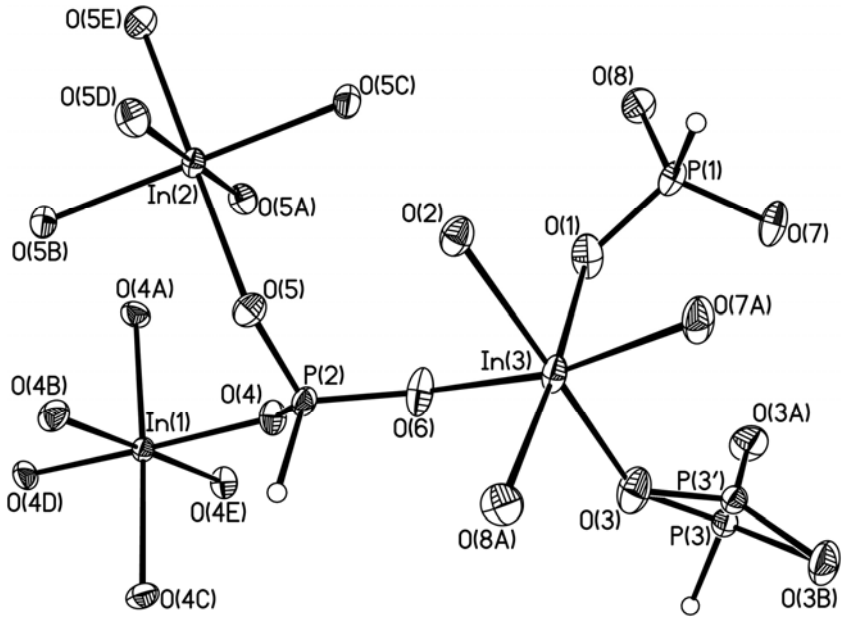
(a)



(b)



(c)



(d)

Fig. S4. The thermal ellipsoid plots (30%) and atomic labelling schemes of (a) InHPO-CJ11, (b) InHPO-CJ12, (c) InHPO-CJ13 and (d) InHPO-CJ14.

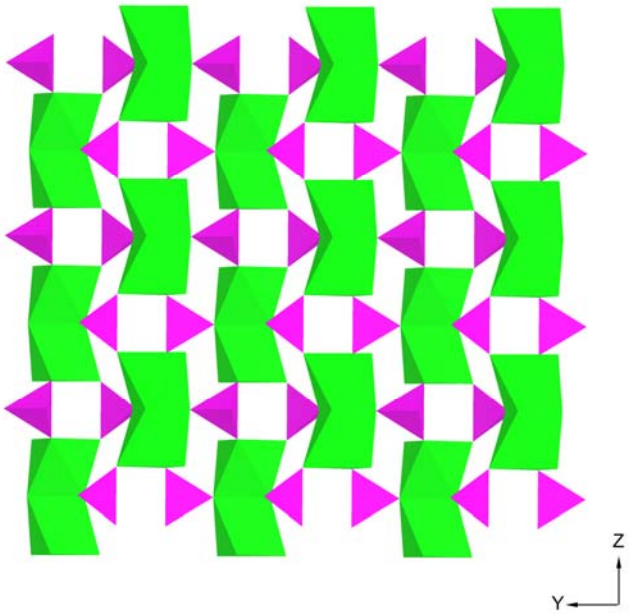
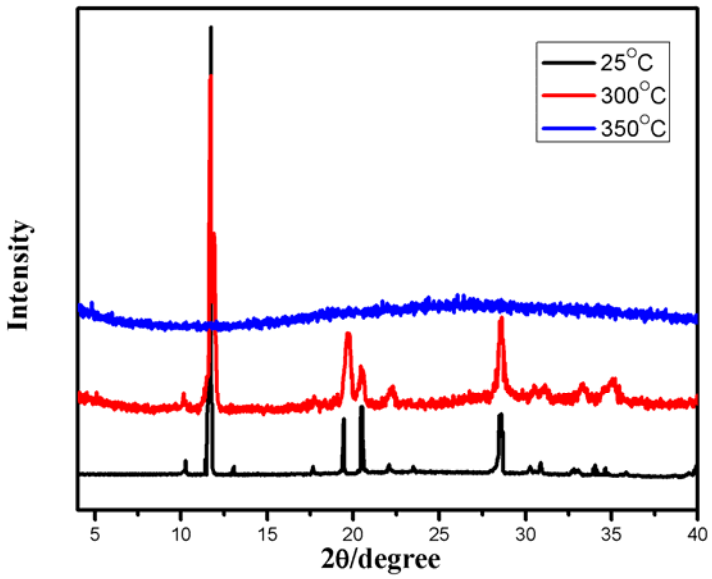
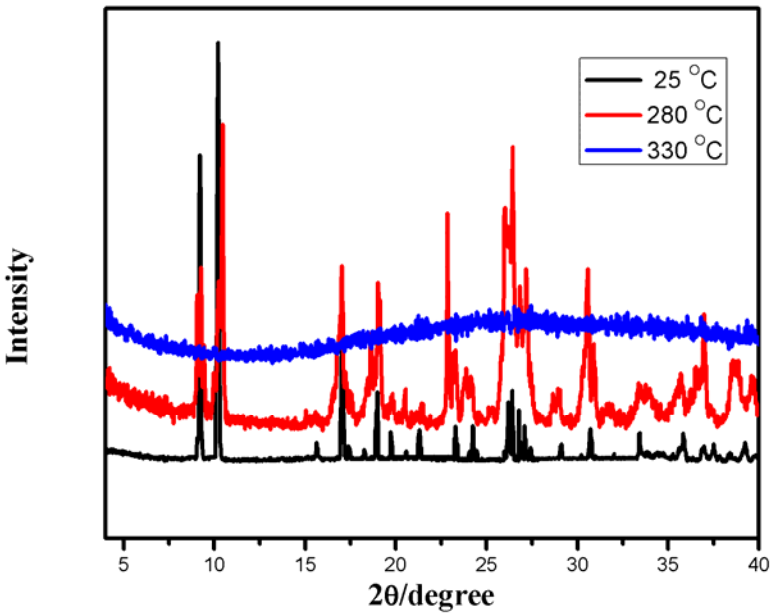


Fig. S5 4-ring layer of InHPO-CJ13 constructed by face-sharing In_2O_{10} dimers and HPO_3 units.

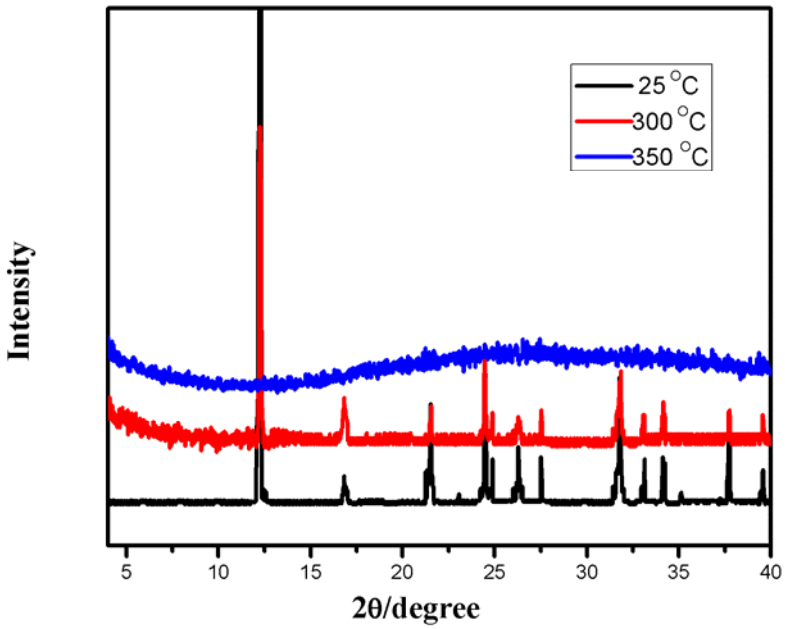
Green, In; pink, P.



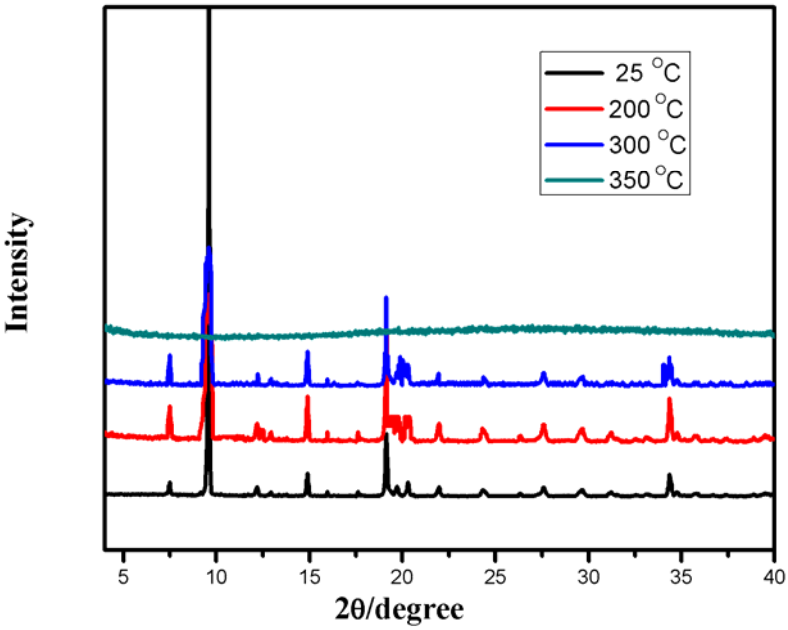
(a)



(b)



(c)



(d)

Figure S6. XRD patterns of (a) InHPO-CJ11, (b) InHPO-CJ12, (c) InHPO-CJ13 and (d) InHPO-CJ14 calcined at different temperatures.