

Supporting Information

Highly Porous Aluminophosphates with Unique Three Dimensional Open Framework Structures from Mild Hydrothermal Syntheses

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Table S1. Important Bond Lengths (angstroms) and Important Bond angles (degrees) for α -NaAlPO₄(OH)(**1**) (a), β -NaAlPO₄(OH)(**2**) (b) and Al_{3.5}P_{5.5}O₁₉(**3**) (c)

Figure S5: TG-DSC curves of α -NaAlPO₄(OH)(**1**) (a), β -NaAlPO₄(OH)(**2**) (b) and Al_{3.5}P_{5.5}O₁₉(**3**) (c).

Figure S6: IR spectra of α -NaAlPO₄(OH)(**1**) (a), β -NaAlPO₄(OH)(**2**) (b) and Al_{3.5}P_{5.5}O₁₉(**3**) (c)

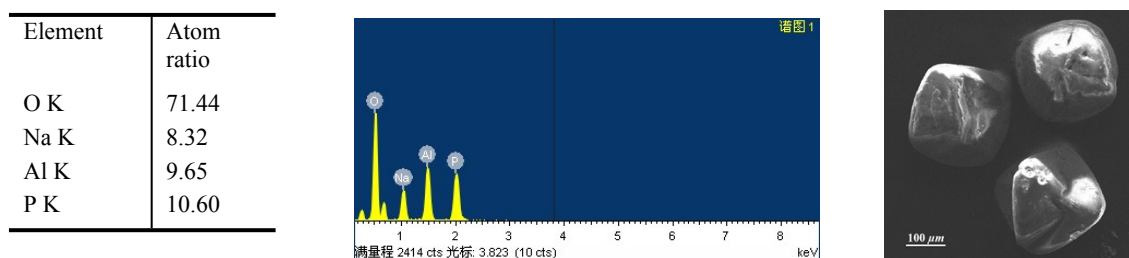


Figure S1: EDX and SEM images of α -NaAlPO₄(OH)(1).

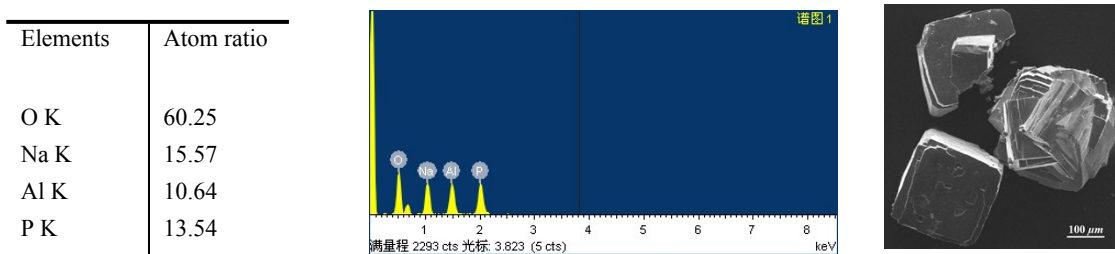


Figure S2: EDX and SEM images of β -NaAlPO₄(OH)(2).

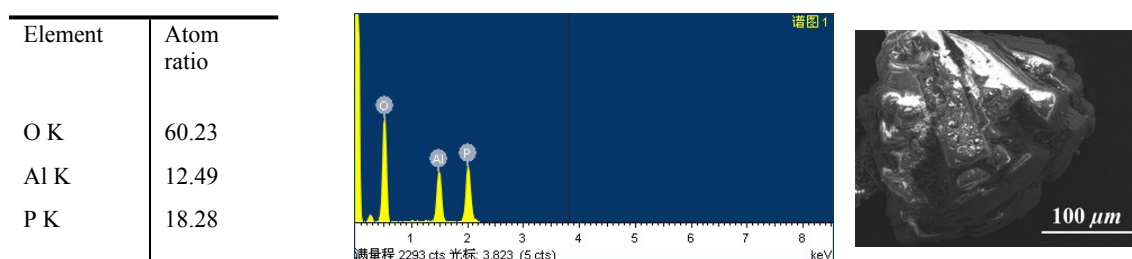


Figure S3: EDX and SEM images of Al_{3.5}P_{5.5}O₁₉(3).

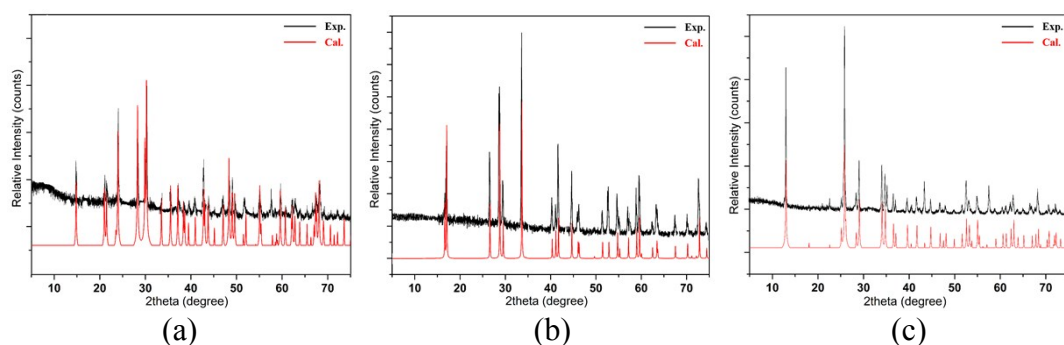


Figure S4: Experimental (black) and simulated (red) PXRD of α -NaAlPO₄(OH)(1) (a), β -NaAlPO₄(OH)(2) (b) and Al_{3.5}P_{5.5}O₁₉(3) (c)

Table S1. Important Bond Lengths (angstroms) and Important Bond angles (degrees) for α -NaAlPO₄(OH)(1), β -NaAlPO₄(OH)(2) and Al_{3.5}P_{5.5}O₁₉(3).

1		2		3	
P(1)-O(2)	1.522(5)	P(1)-O(3)#1	1.527(5)	P(1)-O(3)	1.471(15)
P(1)-O(2)#1	1.522(5)	P(1)-O(3)#2	1.527(5)	P(1)-O(2)#1	1.5104(17)
P(1)-O(3)#1	1.530(5)	P(1)-O(3)#3	1.527(5)	P(1)-O(2)	1.5104(17)
P(1)-O(3)	1.530(5)	P(1)-O(3)	1.527(5)	P(1)-O(1)	1.541(2)
Al(1)-O(2)#6	1.846(6)	Al(1)-O(2)	1.826(10)	Al(1)-O(2)	1.8210(17)
Al(1)-O(2)#1	1.846(6)	Al(1)-O(1)	1.865(4)	Al(1)-O(2)#2	1.8210(17)
Al(1)-O(1)#7	1.849(3)	Al(1)-O(3)	1.884(5)	Al(1)-O(2)#3	1.8210(17)
Al(1)-O(1)	1.849(3)	Al(1)-O(3)#8	1.884(5)	Al(1)-O(1)#4	1.9695(17)
Al(1)-O(3)#3	1.872(5)	Al(1)-O(3)#9	1.884(5)	Al(1)-O(1)#5	1.9695(17)
Al(1)-O(3)#8	1.872(5)	Al(1)-O(3)#10	1.884(5)	Al(1)-O(1)#6	1.9695(17)
O(2)-Na(1)	2.264(18)	O(1)-Na(1)#11	2.472(10)		
O(2)-Na(1)#13	2.43(2)	O(1)-Na(1)#8	2.472(10)	O(3)-P(1)-O(2)#1	107.7(4)
O(3)-Na(1)#5	2.351(14)	O(1)-Na(1)#12	2.472(10)	O(3)-P(1)-O(2)	107.7(4)
O(3)-Na(1)#3	2.549(18)	O(1)-Na(1)	2.472(10)	O(2)#1-P(1)-O(2)	114.26(13)
O(3)-Na(1)	2.708(19)	O(2)-Na(2)#4	2.33(3)	O(3)-P(1)-O(1)	104.6(8)
O(3)-Na(1)#10	2.78(3)	O(2)-Na(2)#13	2.33(3)	O(2)#1-P(1)-O(1)	111.01(8)
Na(1)-O(3)#14	2.351(14)	O(2)-Na(2)#14	2.33(3)	O(2)-P(1)-O(1)	111.01(8)
Na(1)-O(2)#3	2.43(2)	O(2)-Na(2)#15	2.33(3)	O(2)-Al(1)-O(2)#2	98.15(8)
Na(1)-O(3)#13	2.549(18)	O(2)-Na(1)#4	2.428(9)	O(2)-Al(1)-O(2)#3	98.15(8)
Na(1)-O(3)#15	2.78(3)	O(2)-Na(1)#15	2.428(9)	O(2)#2-Al(1)-O(2)#3	98.15(8)
		O(2)-Na(1)#14	2.428(9)	O(2)-Al(1)-O(1)#4	164.87(9)
O(2)-P(1)-O(2)#1	113.5(4)	O(2)-Na(1)#13	2.428(9)	O(2)#2-Al(1)-O(1)#4	91.70(8)
O(2)-P(1)-O(3)#1	111.0(3)	O(3)-Na(1)#11	2.429(6)	O(2)#3-Al(1)-O(1)#4	91.75(8)
O(2)#1-P(1)-O(3)#1	103.9(3)	O(3)-Na(1)	2.429(6)	O(2)-Al(1)-O(1)#5	91.70(8)
O(2)-P(1)-O(3)	103.9(3)	O(3)-Na(2)#5	2.46(2)	O(2)#2-Al(1)-O(1)#5	91.75(8)
O(2)#1-P(1)-O(3)	111.0(3)	O(3)-Na(2)	2.46(2)	O(2)#3-Al(1)-O(1)#5	164.87(9)
O(3)#1-P(1)-O(3)	113.7(4)	Na(1)-O(2)#15	2.428(9)	O(1)#4-Al(1)-O(1)#5	76.47(8)
O(2)#6-Al(1)-O(2)#1	95.0(4)	Na(1)-O(2)#17	2.428(9)	O(2)-Al(1)-O(1)#6	91.75(8)
O(2)#6-Al(1)-O(1)#7	88.42(19)	Na(1)-O(3)#18	2.429(6)	O(2)#2-Al(1)-O(1)#6	164.87(9)
O(2)#1-Al(1)-O(1)#7	176.3(2)	Na(1)-O(3)#8	2.429(6)	O(2)#3-Al(1)-O(1)#6	91.70(8)
O(2)#6-Al(1)-O(1)	176.3(2)	Na(1)-O(3)#19	2.429(6)	O(1)#4-Al(1)-O(1)#6	76.47(8)
O(2)#1-Al(1)-O(1)	88.42(19)	Na(2)-O(2)#17	2.33(3)	O(1)#5-Al(1)-O(1)#6	76.47(8)
O(1)#7-Al(1)-O(1)	88.21(18)	Na(2)-O(2)#15	2.33(3)	O(2)-Al(1)-Al(1)#7	119.25(6)
O(2)#6-Al(1)-O(3)#3	90.7(2)	Na(2)-O(3)#3	2.46(2)	O(2)-Al(1)-Al(1)#7	119.25(6)
O(2)#1-Al(1)-O(3)#3	95.1(2)	Na(2)-O(3)#19	2.46(2)	O(2)-Al(1)-Al(1)#7	119.25(6)
O(1)#7-Al(1)-O(3)#3	86.2(3)	Na(2)-O(3)#5	2.46(2)	O(1)#4-Al(1)-Al(1)#	45.61(5)
O(1)-Al(1)-O(3)#3	87.6(3)			O(1)-Al(1)-Al(1)#7	45.61(5)
O(2)#6-Al(1)-O(3)#8	95.1(2)	O(3)-P(1)-O(3)#2	106.5(4)	O(1)-Al(1)-Al(1)#7	45.61(5)
O(2)#1-Al(1)-O(3)#8	90.7(2)	O(3)-P(1)-O(3)#3	110.98(18)	P(1)-O(3)	1.471(15)

O(1)#7-Al(1)-O(3)#8	87.6(3)	O(3)-P(1)-O(3)#3	110.98(18)	P(1)-O(2)#1	1.5104(17)
		O(3)#1-P(1)-O(3)	110.98(18)	P(1)-O(2)	1.5104(17)
		O(3)#2-P(1)-O(3)	110.98(18)	P(1)-O(1)	1.541(2)
		O(3)#3-P(1)-O(3)	106.5(4)	Al(1)-O(2)	1.8210(17)
		O(2)-Al(1)-O(1)	180	Al(1)-O(2)#2	1.8210(17)
		O(2)-Al(1)-O(3)	95.6(2)	Al(1)-O(2)#3	1.8210(17)
		O(1)-Al(1)-O(3)	84.4(2)	Al(1)-O(1)#4	1.9695(17)
		O(2)-Al(1)-O(3)#8	95.6(2)	Al(1)-O(1)#5	1.9695(17)
		O(1)-Al(1)-O(3)#8	84.4(2)	Al(1)-O(1)#6	1.9695(17)
		O(3)-Al(1)-O(3)#8	89.46(4)		
		O(2)-Al(1)-O(3)#9	95.6(2)	O(3)-P(1)-O(2)#1	107.7(4)
		O(1)-Al(1)-O(3)#9	84.4(2)	O(3)-P(1)-O(2)	107.7(4)
		O(3)-Al(1)-O(3)#9	168.8(4)	O(2)#1-P(1)-O(2)	114.26(13)
		O(3)-Al(1)-O(3)#9	89.46(4)	O(3)-P(1)-O(1)	104.6(8)
		O(2)-Al(1)-O(3)	95.6(2)	O(2)#1-P(1)-O(1)	111.01(8)
		O(1)-Al(1)-O(3)	84.4(2)	O(2)-P(1)-O(1)	111.01(8)
		O(3)-Al(1)-O(3)	89.46(4)	O(2)-Al(1)-O(2)#2	98.15(8)
		O(3)#8-Al(1)-O(3)	168.8(4)	O(2)-Al(1)-O(2)#3	98.15(8)
		O(3)#9-Al(1)-O(3)	89.46(4)	O(2)#2-Al(1)-O(2)#3	98.15(8)

1. Symmetry transformations used to generate equivalent atoms:

#1 $x, y, -z+2$; #2 $x+1/2, -y+3/2, -z+9/4$; #5 $-x+1, -y+2, z-1/2$; #6 $x, y, z-1$; #7 $-x+2, -y+2, z-1/2$; #8 $x+1/2, -y+3/2, -z+5/4$; #9 $-x+3/2, y-1/2, -z+7/4$; #10 $y-1/2, -x+3/2, z-3/4$; #11 $-x+2, -y+2, z+1/2$; #12 $x, y, z+1$; #13 $y-1/2, -x+3/2, z+1/4$; #14 $-x+1, -y+2, z+1/2$; #15 $-y+3/2, x+1/2, z+3/4$

2. Symmetry transformations used to generate equivalent atoms:

#1 $-y+1/2, x-1/2, -z+1/2$; #2 $y+1/2, -x+1/2, -z+1/2$; #3 $-x+1, -y, z$; #4 $-y+1/2, x-1/2, z-1/2$; #5 $-x+1, -y, -z+1$; #6 $x-1/2, y-1/2, z-1/2$; #7 $-y+1, x-1, z$; #8 $-y+1, x, z$; #9 $-x+1, -y+1, z$; #10 $y, -x+1, z$; #11 $y, -x+1, -z+1$; #12 $-x+1, -y+1, -z+1$; #13 $x-1/2, y+1/2, z-1/2$; #14 $y+1/2, -x+3/2, -z+1/2$; #15 $-x+3/2, -y+1/2, -z+1/2$; #16 $y+1, -x+1, -z+1$; #17 $x+1/2, y-1/2, z+1/2$ #18 $-y+1, x, -z+1$

3. Symmetry transformations used to generate equivalent atoms:

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

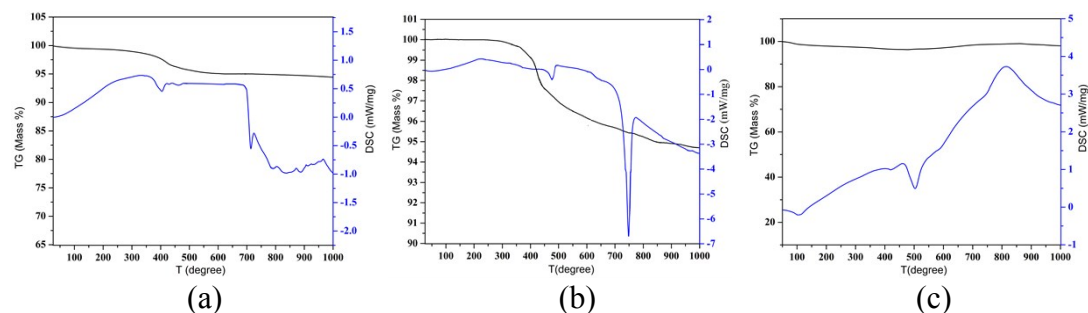


Figure S5: TG-DSC curves of α -NaAlPO₄(OH)(1) (a), β -NaAlPO₄(OH)(2) (b) and Al_{3.5}P_{5.5}O₁₉(3) (c).

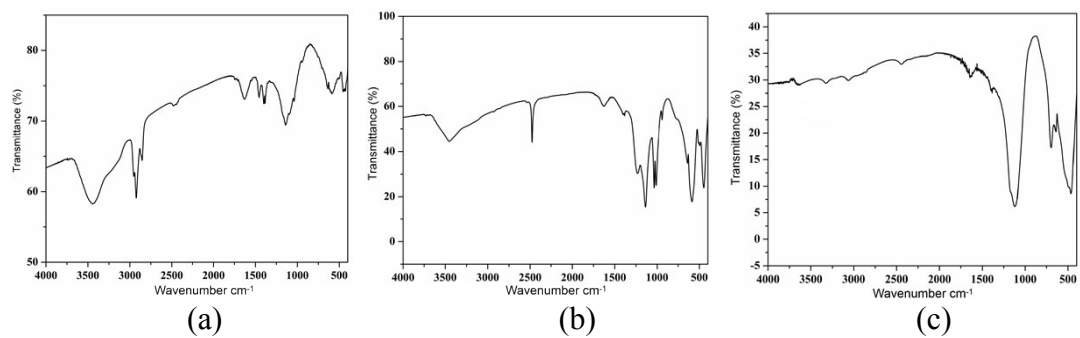


Figure S6: IR spectra of $\alpha\text{-NaAlPO}_4(\text{OH})$ (1) (a), $\beta\text{-NaAlPO}_4(\text{OH})$ (2) (b) and $\text{Al}_{3.5}\text{P}_{5.5}\text{O}_{19}$ (3) (c).