Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

Syntheses and Characterizations of Heteroatom-Containing Open-Framework Aluminophosphates

Yanan Guo, Xiaowei Song, Jiyang Li, Yi Li,* Yide Han, Jihong Yu,* Ruren Xu

E-mail: jihong@jlu.edu.cn; yili@jlu.edu.cn

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry,

Jilin University, Changchun 130012, P. R. China

Tel: (+86) 431-85168608. Fax: (+86) 431-8516-8608.

Table S1 Bond lengths [Å] and angles [deg] for FeAPO-CJ50

Fe(1)-O(14)	1.950(5)	O(1)-Fe(1)-O(2)	179.5(2)
Fe(1)-O(1)	1.959(5)	O(14)-Fe(1)-O(3)	92.9(2)
Fe(1)-O(2)	1.961(5)	O(1)-Fe(1)-O(3)	91.4(2)
Fe(1)-O(3)	2.006(5)	O(2)-Fe(1)-O(3)	88.9(2)
Fe(1)-N(1)	2.075(7)	O(14)-Fe(1)-N(1)	177.5(2)
Fe(1)-N(3)	2.096(7)	O(1)-Fe(1)-N(1)	88.9(2)
Al(1)-O(6)#1	1.728(5)	O(2)-Fe(1)-N(1)	90.7(2)
Al(1)-O(12)#2	1.734(5)	O(3)-Fe(1)-N(1)	85.6(2)
Al(1)-O(4)	1.740(6)	O(14)-Fe(1)-N(3)	89.4(2)
Al(1)-O(5)	1.751(6)	O(1)-Fe(1)-N(3)	90.4(2)
Al(2)-O(15)#3	1.721(5)	O(2)-Fe(1)-N(3)	89.3(2)
Al(2)-O(8)	1.726(5)	O(3)-Fe(1)-N(3)	177.2(2)
Al(2)-O(7)	1.756(5)	N(1)-Fe(1)-N(3)	92.2(3)
Al(2)-O(11)	1.757(5)	O(6)#1-Al(1)-O(12)#2	105.8(3)
Al(3)-O(9)#4	1.717(5)	O(6)#1-Al(1)-O(4)	108.6(3)
Al(3)-O(13)	1.732(6)	O(12)#2-Al(1)-O(4)	115.3(3)
Al(3)-O(10)#5	1.732(6)	O(6)#1-Al(1)-O(5)	110.7(3)
Al(3)-O(16)#5	1.733(5)	O(12)#2-Al(1)-O(5)	108.2(3)
P(1)-O(14)	1.502(5)	O(4)-Al(1)-O(5)	108.2(3)
P(1)-O(5)	1.527(5)	O(15)#3-Al(2)-O(8)	109.2(3)
P(1)-O(7)	1.527(5)	O(15)#3-Al(2)-O(7)	107.3(3)
P(1)-O(6)	1.528(5)	O(8)-Al(2)-O(7)	111.8(3)
P(2)-O(1)	1.494(5)	O(15)#3-Al(2)-O(11)	112.0(3)
P(2)-O(15)	1.523(5)	O(8)-Al(2)-O(11)	108.3(3)
P(2)-O(16)	1.531(5)	O(7)-Al(2)-O(11)	108.4(3)
P(2)-O(4)	1.538(5)	O(9)#4-Al(3)-O(13)	109.7(3)
P(3)-O(3)	1.511(5)	O(9)#4-Al(3)-O(10)#5	109.6(3)
P(3)-O(8)	1.520(5)	O(13)-Al(3)-O(10)#5	107.6(3)
P(3)-O(9)	1.528(5)	O(9)#4-Al(3)-O(16)#5	108.0(3)
P(3)-O(10)	1.537(5)	O(13)-Al(3)-O(16)#5	110.4(3)
P(4)-O(2)	1.500(5)	O(10)#5-Al(3)-O(16)#5	111.7(3)
P(4)-O(12)	1.531(5)	O(14)-P(1)-O(5)	111.5(3)
P(4)-O(13)	1.534(5)	O(14)-P(1)-O(7)	109.8(3)
P(4)-O(11)	1.536(5)	O(5)-P(1)-O(7)	108.1(3)
O(6)-Al(1)#1	1.728(5)	O(14)-P(1)-O(6)	110.7(3)
O(9)-Al(3)#4	1.717(5)	O(5)-P(1)-O(6)	108.4(3)
O(10)-Al(3)#2	1.732(6)	O(7)-P(1)-O(6)	108.1(3)
O(12)-Al(1)#5	1.734(5)	O(1)-P(2)-O(15)	108.7(3)
O(15)-Al(2)#6	1.721(5)	O(1)-P(2)-O(16)	111.9(3)
O(16)-Al(3)#2	1.733(5)	O(15)-P(2)-O(16)	107.3(3)
N(1)-C(3)	1.341(11)	O(1)-P(2)-O(4)	112.4(3)
N(1)-C(1)	1.363(11)	O(15)-P(2)-O(4)	108.1(3)
N(2)-C(3)	1.321(11)	O(16)-P(2)-O(4)	108.3(3)

N(2)-C(2)	1.369(13)	O(3)-P(3)-O(8)	113.6(3)
N(2)-H(2)	0.8600	O(3)-P(3)-O(9)	109.6(3)
N(3)-C(4)	1.313(12)	O(8)-P(3)-O(9)	106.6(3)
N(3)-C(6)	1.353(11)	O(3)-P(3)-O(10)	110.1(3)
N(4)-C(5)	1.304(14)	O(8)-P(3)-O(10)	108.1(3)
N(4)-C(4)	1.323(13)	O(9)-P(3)-O(10)	108.6(3)
N(4)-H(4)	0.8600	O(2)-P(4)-O(12)	111.4(3)
C(1)-C(2)	1.330(13)	O(2)-P(4)-O(13)	110.3(3)
C(1)-H(1)	0.9300	O(12)-P(4)-O(13)	107.7(3)
C(2)-H(2A)	0.9300	O(2)-P(4)-O(11)	112.5(3)
C(3)-H(3)	0.9300	O(12)-P(4)-O(11)	106.8(3)
C(4)-H(4A)	0.9300	O(13)-P(4)-O(11)	107.8(3)
C(5)-C(6)	1.3131	P(2)-O(1)-Fe(1)	141.3(3)
C(5)-H(5)	0.9300	P(4)-O(2)-Fe(1)	148.5(3)
C(6)-H(6)	0.9300	P(3)-O(3)-Fe(1)	135.2(3)
O(14)-Fe(1)-O(1)	89.1(2)	P(2)-O(4)-Al(1)	141.2(4)
O(14)-Fe(1)-O(2)	91.2(2)	P(1)-O(5)-Al(1)	139.1(4)
P(1)-O(6)-Al(1)#1	145.3(4)	P(1)-O(7)-Al(2)	126.9(3)
P(3)-O(8)-Al(2)	144.3(3)	P(3)-O(9)-Al(3)#4	148.9(4)
P(3)-O(10)-Al(3)#2	137.5(4)	P(4)-O(11)-Al(2)	136.8(3)
P(4)-O(12)-Al(1)#5	139.8(4)	P(4)-O(13)-Al(3)	136.7(4)
P(1)-O(14)-Fe(1)	175.3(4)	P(2)-O(15)-Al(2)#6	153.9(4)
P(2)-O(16)-Al(3)#2	152.5(4)	C(3)-N(1)-C(1)	104.0(7)
C(3)-N(1)-Fe(1)	127.3(6)	C(1)-N(1)-Fe(1)	126.4(6)
C(3)-N(2)-C(2)	107.9(8)	C(3)-N(2)-H(2)	126.1
C(2)-N(2)-H(2)	126.1	C(4)-N(3)-C(6)	103.0(8)
C(4)-N(3)-Fe(1)	126.6(7)	C(6)-N(3)-Fe(1)	130.4(6)
C(5)-N(4)-C(4)	105.9(9)	C(5)-N(4)-H(4)	127.1
C(4)-N(4)-H(4)	127.1	C(2)-C(1)-N(1)	111.4(9)
C(2)-C(1)-H(1)	124.3	N(1)-C(1)-H(1)	124.3
C(1)-C(2)-N(2)	105.6(9)	C(1)-C(2)-H(2A)	127.2
N(2)-C(2)-H(2A)	127.2	N(2)-C(3)-N(1)	111.2(8)
N(2)-C(3)-H(3)	124.4	N(1)-C(3)-H(3)	124.4
N(3)-C(4)-N(4)	112.5(10)	N(3)-C(4)-H(4A)	123.7
N(4)-C(4)-H(4A)	123.7	N(4)-C(5)-C(6)	108.7(6)
N(4)-C(5)-H(5)	125.7	C(6)-C(5)-H(5)	125.7
C(5)-C(6)-N(3)	109.9(5)	C(5)-C(6)-H(6)	125.0
N(3)-C(6)-H(6)	125.0		

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

Table S2 Isomer shifts (IS), absolute values of quadrupole splitting (|QS|), full width at full maximum (HWHM) and relative spectral areas (%) of the ^{57}Fe Mössbauer spectroscopy observed at room temperature in FeAPO-CJ50

Name	Cation	IS(mm/s)	QS(mm/s)	HWHM(mm/s)	Area Ratio
FeAPO-CJ50	Fe^{3+}	0.41±0	0.23±0.01	0.38±0	100.0%

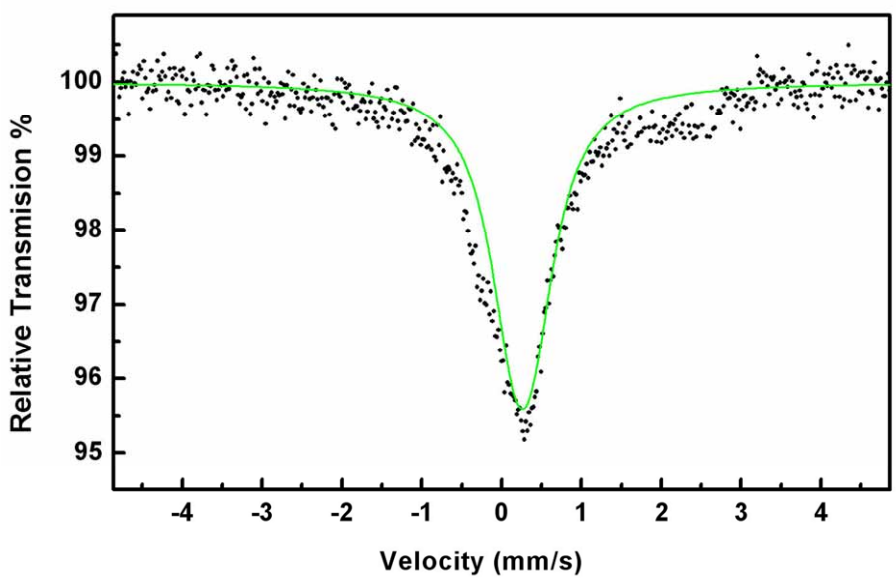

Figure S1 The ^{57}Fe Mössbauer spectroscopy of FeAPO-CJ50 observed at room temperature.