Appendix E: Refinement Data Discussed in Part 3

(1) Refined cell parameters, atomic coordinates and selected bond lengths and angles for calcined Cu-MgAPO STA-6

***a* (Å)**	***b* (Å)**	***c* (Å)**	**Volume (Å^3)**
14.322(1)	14.322(1)	10.200(1)	2092.0(4)

Atom	***x***	***y***	***z***	***Occupancy***	U_{iso} **(x100)**
Al(1)	0.260(2)	0.111(2)	0.000	1	2.0(1)
Al(2)	0.395(1)	-0.105(1)	-0.250	1	2.0(1)
P(1)	0.267(2)	-0.114(2)	0.000	1	2.0(1)
P(2)	0.610(1)	-0.110(1)	-0.250	1	2.0(1)
O(1)	0.234(2)	-0.024(3)	0.000	1	2.4(2)
O(2)	0.337(2)	-0.145(3)	-0.103(2)	1	2.4(2)
O(3)	0.505(2)	-0.127(1)	-0.205(2)	1	2.4(2)
O(4)	0.179(3)	-0.167(3)	0.000	1	2.4(2)
O(5)	0.689(2)	-0.145(2)	-0.143(2)	1	2.4(2)
Cu(1)	0.38(2)	0.87(2)	0.000	0.03(1)	2.0(3)

Bond length (Å)			
Al(1)-O(1)	1.96(4)	P(1)-O(1)	1.37(4)
Al(1)-O(4)	1.65(3)	P(1)-O(2)	1.53(3)
Al(1)-O(5)	1.70(3)	P(1)-O(4)	1.48(5)
Al(2)-O(2)	1.81(2)	P(2)-O(3)	1.59(4)
Al(2)-O(3)	1.67(4)	P(2)-O(5)	1.65(3)
Cu(1)-O(2)	1.25(2)		

O-T-O bond angles (°)			
O(1)-Al(1)-O(4)	115(2)	O(1)-P(1)-O(2)	120(2)
O(1)-Al(1)-O(5)	111(2)	O(1)-P(1)-O(4)	101(3)
O(4)-Al(1)-O(5)	100(2)	O(2)-P(1)-O(2)	90(2)
O(5)-Al(1)-O(5)	118(3)	O(2)-P(1)-O(4)	114(2)
O(2)-Al(2)-O(2)	113(3)	O(3)-P(2)-O(3)	111(2)
O(2)-Al(2)-O(3)	98(1)	O(3)-P(2)-O(5)	114(1)
O(3)-Al(2)-O(3)	115(2)	O(5)-P(2)-O(5)	91(3)

(2) Refined cell parameters, atomic coordinates and selected bond lengths and angles for calcined Cu-SAPO STA-6

***a* (Å)**	***b* (Å)**	***c* (Å)**	**Volume (Å^3)**
14.316(1)	14.316(1)	10.267(1)	2104.2(3)

Atom	***x***	***y***	***z***	***Occupancy***	U_{iso} **(x100)**
Al(1)	0.266(1)	0.107(1)	0.000	1	1.6(2)
Al(2)	0.392(1)	-0.108(1)	-0.250	1	1.6(2)
P(1)	0.263(1)	-0.115(1)	0.000	0.75	1.6(2)
P(2)	0.609(1)	-0.110(1)	-0.250	0.75	1.6(2)
Si(1)	0.263(1)	-0.115(1)	0.000	0.25	1.6(2)
Si(2)	0.609(1)	-0.110(1)	-0.250	0.25	1.6(2)
O(1)	0.241(1)	-0.011(1)	0.000	1	2.9(3)
O(2)	0.323(1)	-0.138(1)	-0.119(1)	1	2.9(3)
O(3)	0.508(1)	-0.126(1)	-0.209(1)	1	2.9(3)
O(4)	0.166(1)	-0.161(1)	0.000	1	2.9(3)
O(5)	0.675(1)	-0.138(1)	-0.138(1)	1	2.9(3)
Cu(1)	0.574(4)	0.52(1)	0.47(1)	0.047(2)	5.1(3)
Cu(2)	0.25(2)	0.25(2)	0.250	0.037(5)	5.1(3)

Bond length (Å)			
Al(1)-O(1)	1.72(1)	P/Si(1)-O(1)	1.53(1)
Al(1)-O(4)	1.73(1)	P/Si(1)-O(2)	1.53(1)
Al(1)-O(5)	1.71(1)	P/Si(1)-O(4)	1.54(1)
Al(2)-O(2)	1.73(1)	P/Si(2)-O(3)	1.53(1)
Al(2)-O(3)	1.73(1)	P/Si(2)-O(5)	1.54(1)
Cu(1)-O(1)	2.4(1)	Cu(2)-O(2)	2.3(4)
Cu(1)-O(4)	2.4(1)	Cu(2)-O(5)	2.3(4)

O-T-O bond angles (^{o})			
O(1)-Al(1)-O(4)	107(1)	O(1)-P/Si(1)-O(2)	109(1)
O(1)-Al(1)-O(5)	111(1)	O(1)-P/Si(1)-O(4)	103(1)
O(4)-Al(1)-O(5)	108(1)	O(2)-P/Si(1)-O(2)	107(1)
O(5)-Al(1)-O(5)	112(1)	O(2)-P/Si(1)-O(4)	114(1)
O(2)-Al(2)-O(2)	108(1)	O(3)-P/Si(2)-O(3)	112(1)
O(2)-Al(2)-O(3)	109.0(4)	O(3)-P/Si(2)-O(5)	109.3(4)
O(3)-Al(2)-O(3)	110(1)	O(5)-P/Si(2)-O(5)	103(1)

(3) Refined cell parameters, atomic coordinates and selected bond lengths and angles for calcined Cu-SAPO STA-7

***a* (Å)**	***b* (Å)**	***c* (Å)**	**Volume (Å^3)**
18.648(5)	18.648(5)	9.405(1)	3270.4(2)

Atom	***x***	***y***	***z***	***Occupancy***	**U_{iso} (x100)**
Al(1)	0.935(1)	0.337(1)	0.419(2)	1	0.8(1)
Al(2)	0.826(1)	0.545(1)	0.344(2)	1	0.8(1)
Al(3)	1.055(1)	0.567(1)	0.171(3)	1	0.8(1)
P(1)	0.833(1)	0.436(1)	0.597(2)	0.75	0.8(1)
P(2)	0.953(1)	0.661(1)	0.344(2)	0.75	0.8(1)
P(3)	0.934(1)	0.447(1)	0.171(2)	0.75	0.8(1)
Si(1)	0.833(1)	0.436(1)	0.597(2)	0.25	0.8(1)
Si(2)	0.953(1)	0.661(1)	0.344(2)	0.25	0.8(1)
Si(3)	0.934(1)	0.447(1)	0.171(2)	0.25	0.8(1)
O(1)	0.865(1)	0.369(1)	0.521(4)	1	1.8(2)
O(2)	0.940(2)	0.378(1)	0.257(3)	1	1.8(2)
O(3)	0.922(1)	0.248(1)	0.391(3)	1	1.8(2)
O(4)	0.841(2)	0.502(1)	0.508(2)	1	1.8(2)
O(5)	0.863(1)	0.441(2)	0.747(2)	1	1.8(2)
O(6)	0.862(2)	0.486(1)	0.216(3)	1	1.8(2)
O(7)	0.880(1)	0.621(1)	0.345(3)	1	1.8(2)
O(8)	0.738(1)	0.566(1)	0.329(3)	1	1.8(2)
O(9)	1.002(2)	0.645(1)	0.208(3)	1	1.8(2)
O(10)	0.986(1)	0.641(1)	0.494(3)	1	1.8(2)
O(11)	1.005(1)	0.490(1)	0.198(2)	1	1.8(2)
O(12)	0.923(2)	0.426(2)	0.012(2)	1	1.8(2)
Cu(1)	0.686(3)	0.26(1)	0.44(1)	0.09(1)	3.6(3)
Cu(2)	0.22(1)	0.184(4)	0.66(1)	0.09(1)	3.6(3)
Cu(3)	0.25(4)	0.01(1)	0.25(3)	0.03(1)	3.6(3)

Bond length (Å)					
Al(1)-O(1)	1.72(2)	P/Si(1)-O(1)	1.56(2)	Cu(1)-O(1)	2.2(2)
Al(1)-O(2)	1.72(2)	P/Si(1)-O(3)	1.53(2)	Cu(1)-O(3)	2.1(2)
Al(1)-O(3)	1.70(2)	P/Si(1)-O(4)	1.49(2)		
Al(1)-O(10)	1.73(2)	P/Si(1)-O(5)	1.52(2)	Cu(2)-O(7)	2.3(1)
				Cu(2)-O(8)	2.2(1)
Al(2)-O(4)	1.78(2)	P/Si(2)-O(7)	1.55(2)		
Al(2)-O(6)	1.76(2)	P/Si(2)-O(8)	1.48(2)	Cu(3)-O(3)	2.1(3)
Al(2)-O(7)	1.74(2)	P/Si(2)-O(9)	1.60(2)	Cu(3)-O(5)	2.6(1)
Al(2)-O(8)	1.70(2)	P/Si(2)-O(10)	1.58(2)		
Al(3)-O(5)	1.72(2)	P/Si(3)-O(2)	1.52(2)		
Al(3)-O(9)	1.79(2)	P/Si(3)-O(6)	1.58(2)		
Al(3)-O(11)	1.74(2)	P/Si(3)-O(11)	1.58(2)		
Al(3)-O(12)	1.77(2)	P/Si(3)-O(12)	1.56(2)		

O-T-O bond angles (^{o})					
O(1)-Al(1)-O(2)	112(2)	O(5)-Al(3)-O(9)	119(2)	O(7)-P/Si(2)-O(8)	105(2)
O(1)-Al(1)-O(3)	109(2)	O(5)-Al(3)-O(11)	110(2)	O(7)-P/Si(2)-O(9)	114(2)
O(1)-Al(1)-O(10)	107(2)	O(5)-Al(3)-O(12)	104(2)	O(7)-P/Si(2)-O(10)	103(2)
O(2)-Al(1)-O(3)	108(1)	O(9)-Al(3)-O(11)	110(2)	O(8)-P/Si(2)-O(9)	104(2)
O(2)-Al(1)-O(10)	105(1)	O(9)-Al(3)-O(12)	105(2)	O(8)-P/Si(2)-O(10)	114(2)
O(3)-Al(1)-O(10)	115(2)	O(11)-Al(3)-O(12)	109(2)	O(9)-P/Si(2)-O(10)	116(2)
O(4)-Al(2)-O(6)	105(2)	O(1)-P/Si(1)-O(3)	107(2)	O(2)-P/Si(3)-O(6)	108(2)
O(4)-Al(2)-O(7)	106(1)	O(1)-P/Si(1)-O(4)	111(2)	O(2)-P/Si(3)-O(11)	105(2)
O(4)-Al(2)-O(8)	109(2)	O(1)-P/Si(1)-O(5)	109(2)	O(2)-P/Si(3)-O(12)	108(2)
O(6)-Al(2)-O(7)	107(1)	O(3)-P/Si(1)-O(4)	106(2)	O(6)-P/Si(3)-O(11)	116(2)
O(6)-Al(2)-O(8)	117(1)	O(3)-P/Si(1)-O(5)	108(2)	O(6)-P/Si(3)-O(12)	106(2)
O(7)-Al(2)-O(8)	112(1)	O(4)-P/Si(1)-O(5)	116(2)	O(11)-P/Si(3)-O(12)	113(2)

(4) Refined cell parameters, atomic coordinates and selected bond lengths and angles for calcined Cu-MgAPO-18

***a* (Å)**	***b* (Å)**	***c* (Å)**	***β* (°)**	**Volume (Å^3)**
13.533(2)	12.678(3)	18.435(5)	87.70(3)	3163(1)

Atom	***x***	***y***	***z***	***Occupancy***	**U_{iso} (x100)**
Al(1)	0.116(1)	0.050(1)	0.167(1)	1	6.4(3)
Al(2)	0.122(1)	-0.218(1)	0.943(1)	1	6.4(3)
Al(3)	-0.224(1)	-0.092(1)	0.049(1)	1	6.4(3)
P(1)	0.223(1)	-0.097(1)	0.055(1)	1	6.4(3)
P(2)	-0.113(1)	-0.233(1)	0.929(1)	1	6.4(3)
P(3)	-0.116(1)	0.026(1)	0.159(1)	1	6.4(3)
O(1)	-0.166(2)	-0.072(2)	0.131(1)	1	7.2(1)
O(2)	-0.144(2)	-0.164(3)	-0.007(1)	1	7.2(1)
O(3)	-0.002(1)	-0.251(2)	0.932(2)	1	7.2(1)
O(4)	0.138(2)	-0.169(3)	0.030(1)	1	7.2(1)
O(5)	0.195(2)	-0.033(2)	0.121(1)	1	7.2(1)
O(6)	-0.005(1)	0.017(2)	0.144(2)	1	7.2(1)
O(7)	-0.157(2)	0.124(2)	0.121(1)	1	7.2(1)
O(8)	-0.333(2)	-0.161(2)	0.064(2)	1	7.2(1)
O(9)	0.134(2)	0.037(2)	0.260(1)	1	7.2(1)
O(10)	0.189(2)	-0.332(2)	0.927(2)	1	7.2(1)
O(11)	-0.140(2)	-0.180(1)	0.858(1)	1	7.2(1)
O(12)	-0.253(2)	0.027(2)	1.008(1)	1	7.2(1)
Cu(1)	0.43(1)	0.84(1)	0.508(3)	0.22(2)	2.5(2)

Bond length (Å)					
Al(1)-O(5)	1.73(1)	Al(3)-O(1)	1.73(1)	P(2)-O(2)	1.53(1)
Al(1)-O(6)	1.75(1)	Al(3)-O(2)	1.74(1)	P(2)-O(3)	1.52(1)
Al(1)-O(9)	1.74(1)	Al(3)-O(8)	1.74(1)	P(2)-O(8)	1.53(1)
Al(1)-O(11)	1.74(1)	Al(3)-O(12)	1.72(1)	P(2)-O(11)	1.53(1)
Al(2)-O(3)	1.74(1)	P(1)-O(4)	1.54(1)	P(3)-O(1)	1.51(1)
Al(2)-O(4)	1.74(1)	P(1)-O(5)	1.51(1)	P(3)-O(6)	1.53(1)
Al(2)-O(7)	1.74(1)	P(1)-O(10)	1.53(1)	P(3)-O(7)	1.53(1)
Al(2)-O(10)	1.73(1)	P(1)-O(12)	1.52(1)	P(3)-O(9)	1.53(1)
		Cu(1)-O(3)	2.1(1)	Cu(1)-O(8)	1.9(1)

O-T-O bond angles (^{o})					
O(5)-Al(1)-O(6)	108(1)	O(1)-Al(3)-O(2)	108(1)	O(2)-P(2)-O(3)	110(1)
O(5)-Al(1)-O(9)	110(1)	O(1)-Al(3)-O(8)	109(1)	O(2)-P(2)-O(8)	108(1)
O(5)-Al(1)-O(11)	109(1)	O(1)-Al(3)-O(12)	110(1)	O(2)-P(2)-O(11)	110(1)
O(6)-Al(1)-O(9)	111(1)	O(2)-Al(3)-O(8)	111(1)	O(3)-P(2)-O(8)	110(1)
O(6)-Al(1)-O(11)	109(1)	O(2)-Al(3)-O(12)	110(1)	O(3)-P(2)-O(11)	109(1)
O(9)-Al(1)-O(11)	109(1)	O(8)-Al(3)-O(12)	109(1)	O(8)-P(2)-O(11)	109(1)
O(3)-Al(2)-O(4)	109(1)	O(4)-P(1)-O(5)	112(1)	O(1)-P(3)-O(6)	108(1)
O(3)-Al(2)-O(7)	110(1)	O(4)-P(1)-O(10)	107(1)	O(1)-P(3)-O(7)	110(1)
O(3)-Al(2)-O(10)	107(1)	O(4)-P(1)-O(12)	108(1)	O(1)-P(3)-O(9)	110(1)
O(4)-Al(2)-O(7)	110(1)	O(5)-P(1)-O(10)	109(1)	O(6)-P(3)-O(7)	109(1)
O(4)-Al(2)-O(10)	112(1)	O(5)-P(1)-O(12)	111(1)	O(6)-P(3)-O(9)	110(1)
O(7)-Al(2)-O(10)	108(1)	O(10)-P(1)-O(12)	109(1)	O(7)-P(3)-O(9)	109(1)

(5) Refined cell parameters, atomic coordinates and selected bond lengths and angles for calcined Cu-MgAPO-5

***a* (Å)**	***b* (Å)**	***c* (Å)**	***β* (°)**	**Volume (Å^3)**
13.687(1)	13.687(1)	8.3145(5)	120	1348.9(1)

Atom	***x***	***y***	***z***	***Occupancy***	**U_{iso} (x100)**
Al(1)	0.329(2)	0.458(1)	0.093(1)	1	4.8(2)
P(1)	0.118(2)	0.450(1)	0.218(2)	1	4.8(2)
O(1)	0.194(2)	0.418(1)	0.138(3)	1	8.1(4)
O(2)	-0.004(2)	0.357(1)	0.176(3)	1	8.1(4)
O(3)	0.122(2)	0.459(2)	0.392(2)	1	8.1(4)
O(4)	0.158(2)	0.570(2)	0.162(4)	1	8.1(4)

Bond length (Å)			
Al(1)-O(1)	1.69(2)	P(1)-O(1)	1.48(2)
Al(1)-O(2)	1.69(2)	P(1)-O(2)	1.56(2)
Al(1)-O(3)	1.68(2)	P(1)-O(3)	1.45(2)
Al(1)-O(4)	1.72(3)	P(1)-O(4)	1.51(2)

O-T-O bond angles (°)			
O(1)-Al(1)-O(2)	108(1)	O(1)-P(1)-O(2)	106(2)
O(1)-Al(1)-O(3)	110(1)	O(1)-P(1)-O(3)	118(2)
O(1)-Al(1)-O(4)	109(1)	O(1)-P(1)-O(4)	104(2)
O(2)-Al(1)-O(3)	111(1)	O(2)-P(1)-O(3)	106(2)
O(2)-Al(1)-O(4)	109(1)	O(2)-P(1)-O(4)	119(2)
O(3)-Al(1)-O(4)	109(1)	O(3)-P(1)-O(4)	104(2)