

Electronic Supplementary Information

A New Magnesium-Containing Aluminophosphate with Zeolite-Like Structure

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Table S1. The bond lengths [Å] and angles [deg] for JU96.

Mg(1)-O(6)	1.999(3)	P(2)-O(11)	1.527(3)
Mg(1)-O(12)#1	2.026(3)	P(2)-O(5)	1.535(3)
Mg(1)-O(17)	2.073(3)	P(2)-O(4)	1.544(3)
Mg(1)-O(16)	2.098(3)	P(3)-O(12)	1.487(3)
Mg(1)-O(2)	2.109(3)	P(3)-O(8)	1.527(3)
Mg(1)-O(18)	2.236(3)	P(3)-O(14)	1.539(3)
Al(1)-O(13)#2	1.722(3)	P(3)-O(1)	1.548(3)
Al(1)-O(7)	1.726(3)	P(4)-O(17)	1.483(3)
Al(1)-O(15)#3	1.734(3)	P(4)-O(9)	1.525(3)
Al(1)-O(14)#4	1.740(3)	P(4)-O(13)	1.532(3)
Al(2)-O(9)	1.715(3)	P(4)-O(15)	1.540(3)
Al(2)-O(5)#5	1.726(3)	O(5)-Al(2)#1	1.726(3)
Al(2)-O(1)	1.745(3)	O(8)-Al(3)#8	1.726(3)
Al(2)-O(4)	1.746(3)	O(10)-Al(3)#9	1.736(3)
Al(3)-O(11)#6	1.715(3)	O(11)-Al(3)#10	1.715(3)
Al(3)-O(8)#4	1.726(3)	O(12)-Mg(1)#5	2.026(3)
Al(3)-O(10)#7	1.736(3)	O(13)-Al(1)#11	1.722(3)
Al(3)-O(3)	1.751(3)	O(14)-Al(1)#8	1.740(3)
P(1)-O(2)	1.503(3)	O(15)-Al(1)#3	1.734(3)
P(1)-O(7)	1.525(3)	N(1)-C(3)	1.470(6)
P(1)-O(10)	1.542(3)	N(1)-C(2)	1.504(6)
P(1)-O(3)	1.543(3)	C(2)-C(3)#12	1.486(7)
P(2)-O(6)	1.483(3)	C(3)-C(2)#12	1.486(7)
O(6)-Mg(1)-O(12)#1	97.30(13)	O(10)-P(1)-O(3)	107.19(16)
O(6)-Mg(1)-O(17)	92.87(13)	O(6)-P(2)-O(11)	111.68(17)
O(12)#1-Mg(1)-O(17)	90.72(13)	O(6)-P(2)-O(5)	113.24(16)
O(6)-Mg(1)-O(16)	171.54(14)	O(11)-P(2)-O(5)	107.71(17)
O(12)#1-Mg(1)-O(16)	91.11(13)	O(6)-P(2)-O(4)	111.11(17)
O(17)-Mg(1)-O(16)	86.13(14)	O(11)-P(2)-O(4)	107.49(16)
O(6)-Mg(1)-O(2)	89.29(12)	O(5)-P(2)-O(4)	105.23(16)
O(12)#1-Mg(1)-O(2)	96.51(12)	O(12)-P(3)-O(8)	113.43(16)
O(17)-Mg(1)-O(2)	172.14(14)	O(12)-P(3)-O(14)	111.31(17)
O(16)-Mg(1)-O(2)	90.63(13)	O(8)-P(3)-O(14)	108.26(17)
O(6)-Mg(1)-O(18)	87.84(13)	O(12)-P(3)-O(1)	112.14(16)
O(12)#1-Mg(1)-O(18)	174.84(14)	O(8)-P(3)-O(1)	105.58(16)
O(17)-Mg(1)-O(18)	88.61(13)	O(14)-P(3)-O(1)	105.65(15)
O(16)-Mg(1)-O(18)	83.74(14)	O(17)-P(4)-O(9)	112.49(18)
O(2)-Mg(1)-O(18)	83.91(12)	O(17)-P(4)-O(13)	112.25(19)
O(13)#2-Al(1)-O(7)	108.33(15)	O(9)-P(4)-O(13)	108.06(17)

O(13)#2-Al(1)-O(15)#3	107.65(14)	O(17)-P(4)-O(15)	111.79(18)
O(7)-Al(1)-O(15)#3	110.02(14)	O(9)-P(4)-O(15)	106.27(16)
O(13)#2-Al(1)-O(14)#4	110.33(15)	O(13)-P(4)-O(15)	105.55(16)
O(7)-Al(1)-O(14)#4	110.55(15)	P(3)-O(1)-Al(2)	136.62(19)
O(15)#3-Al(1)-O(14)#4	109.90(14)	P(1)-O(2)-Mg(1)	137.41(16)
O(9)-Al(2)-O(5)#5	108.87(15)	P(1)-O(3)-Al(3)	141.95(19)
O(9)-Al(2)-O(1)	109.75(14)	P(2)-O(4)-Al(2)	131.81(18)
O(5)#5-Al(2)-O(1)	113.88(14)	P(2)-O(5)-Al(2)#1	146.05(19)
O(9)-Al(2)-O(4)	110.67(15)	P(2)-O(6)-Mg(1)	141.10(18)
O(5)#5-Al(2)-O(4)	109.99(15)	P(1)-O(7)-Al(1)	141.98(19)
O(1)-Al(2)-O(4)	103.60(14)	P(3)-O(8)-Al(3)#8	150.4(2)
O(11)#6-Al(3)-O(8)#4	109.96(15)	P(4)-O(9)-Al(2)	155.0(2)
O(11)#6-Al(3)-O(10)#7	109.41(15)	P(1)-O(10)-Al(3)#9	138.26(18)
O(8)#4-Al(3)-O(10)#7	110.67(14)	P(2)-O(11)-Al(3)#10	171.6(2)
O(11)#6-Al(3)-O(3)	107.81(15)	P(3)-O(12)-Mg(1)#5	150.21(19)
O(8)#4-Al(3)-O(3)	109.25(15)	P(4)-O(13)-Al(1)#11	139.7(2)
O(10)#7-Al(3)-O(3)	109.68(14)	P(3)-O(14)-Al(1)#8	138.69(18)
O(2)-P(1)-O(7)	111.73(16)	P(4)-O(15)-Al(1)#3	136.15(18)
O(2)-P(1)-O(10)	112.61(16)	P(4)-O(17)-Mg(1)	148.0(2)
O(7)-P(1)-O(10)	107.28(16)	C(3)-N(1)-C(2)	110.8(3)
O(2)-P(1)-O(3)	108.64(15)	C(3)#12-C(2)-N(1)	110.2(4)
O(7)-P(1)-O(3)	109.24(16)	N(1)-C(3)-C(2)#12	110.4(4)

For JU96 Symmetry transformations used to generate equivalent atoms:

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