Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Two New Four-Connected Zeolite-like Magnesium Aluminophosphates with Intersecting 8-Ring Channels

*Yanyan Wang, Ying Mu, Yanjun Sun and Jiyang Li**

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry,

College of Chemistry, Jilin University, Changchun 130012, P. R. China

Table S1. Crystal data and structure refinement for JU94 and JU95[a].

compounds	JU94	JU95
empirical formula	$MgAl_3P_4O_{18}C_2H_{10}N$	$MgAl_3P_4O_{18}C_2H_{10}N$
formula weight	565.24	565.24
temperature	296(2) K	293(2) K
wavelength(Å)	0.71073	0.71073
crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
unit cell dimensions		
a (Å)	12.3675(4)	8.1871(16)
b (Å)	14.9405(5)	14.690(3)
c (Å)	9.1706(3)	14.096(3)
α (deg)	90	90
β (deg)	98.4930(10)	92.24(3)
γ (deg)	90	90
volume(Å^3)	1675.93(10)	1694.0(6)
Z, calculated density(mg/m^3)	4, 2.240	4, 2.216
absorption coefficient(mm^{-1})	0.746	0.738
F(000)	1136	1136
crystal size(mm^3)	0.21 × 0.15 × 0.14	0.10 × 0.10 × 0.10
θ range(°) for data collection	1.66–28.37	3.13–27.47
limiting indices	$-13 \le h \le 16$, $-18 \le k \le 19$, $-12 \le l \le 10$	$-10 \le h \le 10$, $-19 \le k \le 17$, $-18 \le l \le 18$
reflections collected/unique	12289/4187, [R(int) = 0.0315]	15881/3818, [R(int) = 0.0255]
completeness to θ (%)	28.37, 99.9	27.47, 98.2
absorption correction	semi-empirical from equivalents	semi-empirical from equivalents
max and min transmission	0.9027 and 0.8591	0.9298 and 0.9298
refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2
data/restraints/parameters	4187/0/271	3818/0/262
goodness-of-fit on F^2	1.069	1.080
final R indices [$I > 2\,\sigma\,(I)$]	$R_1 = 0.0364$, $wR_2 = 0.1024$	$R_1 = 0.0342$, $wR_2 = 0.0951$
R indices (all data)	$R_1 = 0.0461$, $wR_2 = 0.1093$	$R_1 = 0.0372$, $wR_2 = 0.0964$
largest diff. peak and hole (eÅ^{-3})	0.880 and -0.483	0. 639 and -0.573

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

Table S2. Crystal data and structure refinement for JU94-400 and JU95-300[a].

compounds	JU94-400	JU95-300
empirical formula	$MgAl_3P_4O_{17}C_2H_8N$	$MgAl_3P_4O_{16}C_2H_6N$
formula weight	547.22	529.21
temperature	296(2) K	296(2) K
wavelength(Å)	0.71073	0.71073
crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
unit cell dimensions		
a (Å)	12.389(5)	8.3877(14)
b (Å)	14.923(6)	14.399(2)
c (Å)	9.386(4)	14.017(2)
α (deg)	90	90
β (deg)	98.699(7)	91.552(3)
γ (deg)	90	90
volume(Å^3)	1715.2(12)	1692.4(5)
Z, calculated density(mg/m^3)	4, 2.119	4, 2.077
absorption coefficient(mm^{-1})	0.721	0.723
F(000)	1096	1056
crystal size(mm^3)	0.20 × 0.12 × 0.10	0.30 × 0.20 × 0.05
θ range(°) for data collection	1.66–29.39	2.03–28.27
limiting indices	$-8 \le h \le 17$, $-20 \le k \le 20$, $-12 \le l \le 12$	$-10 \le h \le 11$, $-16 \le k \le 19$, $-18 \le l \le 18$
reflections collected/unique	13511/4653, [R(int) = 0.0681]	13543/4196, [R(int) = 0.0391]
completeness to θ (%)	29.39, 98.5	28.27, 99.9
absorption correction	semi-empirical from equivalents	semi-empirical from equivalents
max and min transmission	0.9314 and 0.8692	0.9648 and 0.8123
refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2
data/restraints/parameters	4653/0/253	4196/0/244
goodness-of-fit on F^2	1.120	1.123
final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0950$, $wR_2 = 0.2521$	$R_1 = 0.0497$, $wR_2 = 0.1248$
R indices (all data)	$R_1 = 0.1289$, $wR_2 = 0.2681$	$R_1 = 0.0629$, $wR_2 = 0.1310$
largest diff. peak and hole (eÅ^{-3})	1.804 and -0.809	1.335 and -0.506

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w = 1/\sigma^2(F_o^2)$.

Table S3. Selected bond lengths [Å] and angles [deg] for JU94 and JU94-400.

JU94		JU94-400	
Mg(1)-O(10)#1	2.033(2)	Mg(1)-O(16)#7	1.971(7)
Mg(1)-O(12)#1	2.052(2)	Mg(1)-O(14)	2.002(7)
Mg(1)-O(9)#1	2.065(2)	Mg(1)-O(5)	2.016(7)
Mg(1)-O(4)	2.075(2)	Mg(1)-O(6)	2.060(7)
Mg(1)-O(18)	2.085(2)	Mg(1)-O(17)	2.098(8)
Mg(1)-O(17)	2.232(3)	Al(1)-O(7)	1.738(6)
Al(1)-O(14)#2	1.720(2)	Al(1)-O(10)#1	1.740(6)
Al(1)-O(5)#1	1.730(2)	Al(1)-O(4)	1.747(6)
Al(1)-O(2)#3	1.740(2)	Al(1)-O(1)	1.750(6)
Al(1)-O(6)	1.741(2)	Al(2)-O(11)#2	1.721(6)
Al(2)-O(16)	1.732(2)	Al(2)-O(13)#3	1.737(6)
Al(2)-O(3)	1.732(2)	Al(2)-O(2)#3	1.742(6)
Al(2)-O(15)#4	1.734(2)	Al(2)-O(3)	1.746(6)
Al(2)-O(13)	1.746(2)	Al(3)-O(15)#4	1.716(7)
Al(3)-O(1)#5	1.716(2)	Al(3)-O(9)#5	1.743(7)
Al(3)-O(11)	1.733(2)	Al(3)-O(8)#6	1.753(7)
Al(3)-O(8)#6	1.734(2)	Al(3)-O(12)	1.758(6)
Al(3)-O(7)	1.736(2)	P(1)-O(14)	1.506(6)
P(1)-O(4)	1.496(2)	P(1)-O(4)	1.544(6)
P(1)-O(16)	1.528(2)	P(1)-O(11)	1.545(6)
P(1)-O(14)	1.532(2)	P(1)-O(10)	1.550(6)
P(1)-O(6)	1.541(2)	P(2)-O(6)	1.512(6)
P(2)-O(12)	1.501(2)	P(2)-O(8)	1.520(6)
P(2)-O(5)	1.527(2)	P(2)-O(3)	1.531(6)
P(2)-O(8)	1.528(2)	P(2)-O(2)	1.551(6)
P(2)-O(11)	1.540(2)	P(3)-O(16)	1.500(7)
P(3)-O(10)	1.488(2)	P(3)-O(7)	1.512(6)
P(3)-O(3)	1.535(2)	P(3)-O(15)	1.521(7)
P(3)-O(1)	1.536(2)	P(3)-O(9)	1.547(7)
P(3)-O(15)	1.537(2)	P(4)-O(5)	1.498(6)
P(4)-O(9)	1.486(2)	P(4)-O(12)	1.533(6)
P(4)-O(2)	1.540(2)	P(4)-O(1)	1.549(6)
P(4)-O(13)	1.543(2)	P(4)-O(13)	1.562(6)
P(4)-O(7)	1.545(2)	N(1)-C(1)	1.476(14)
N(1)-C(1)	1.408(5)	N(1)-C(2)	1.491(16)
N(1)-C(2)	1.620(6)	C(1)-C(2)#11	1.549(16)
C(1)-C(2)#9	1.506(6)	C(2)-C(1)#11	1.549(16)
C(1)-N(2)	1.654(9)		
C(2)-N(2)	1.446(9)		
O(10)#1-Mg(1)-O(12)#1	90.51(9)	O(14)-P(1)-O(4)	112.8(4)
O(10)#1-Mg(1)-O(9)#1	95.02(10)	O(14)-P(1)-O(11)	109.7(4)

O(12)#1-Mg(1)-O(9)#1	93.76(9)	O(4)-P(1)-O(11)	108.6(4)
O(10)#1-Mg(1)-O(4)	167.94(10)	O(14)-P(1)-O(10)	110.9(4)
O(12)#1-Mg(1)-O(4)	92.12(9)	O(4)-P(1)-O(10)	107.0(3)
O(9)#1-Mg(1)-O(4)	96.55(9)	O(11)-P(1)-O(10)	107.6(4)
O(10)#1-Mg(1)-O(18)	89.95(10)	O(6)-P(2)-O(8)	113.6(4)
O(12)#1-Mg(1)-O(18)	176.73(10)	O(6)-P(2)-O(3)	108.6(4)
O(9)#1-Mg(1)-O(18)	89.43(10)	O(8)-P(2)-O(3)	110.9(4)
O(4)-Mg(1)-O(18)	86.78(9)	O(6)-P(2)-O(2)	110.3(4)
O(10)#1-Mg(1)-O(17)	82.35(10)	O(8)-P(2)-O(2)	106.0(4)
O(12)#1-Mg(1)-O(17)	89.29(10)	O(3)-P(2)-O(2)	107.3(4)
O(9)#1-Mg(1)-O(17)	176.00(10)	O(16)-P(3)-O(7)	112.7(4)
O(4)-Mg(1)-O(17)	85.92(10)	O(16)-P(3)-O(15)	111.6(4)
O(18)-Mg(1)-O(17)	87.57(10)	O(7)-P(3)-O(15)	107.2(4)
O(14)#2-Al(1)-O(5)#1	111.40(12)	O(16)-P(3)-O(9)	111.5(4)
O(14)#2-Al(1)-O(2)#3	103.61(11)	O(7)-P(3)-O(9)	106.3(4)
O(5)#1-Al(1)-O(2)#3	110.29(11)	O(15)-P(3)-O(9)	107.2(4)
O(14)#2-Al(1)-O(6)	113.58(12)	O(5)-P(4)-O(12)	112.3(4)
O(5)#1-Al(1)-O(6)	108.88(11)	O(5)-P(4)-O(1)	113.5(3)
O(2)#3-Al(1)-O(6)	108.95(12)	O(12)-P(4)-O(1)	105.7(3)
O(16)-Al(2)-O(3)	111.50(11)	O(5)-P(4)-O(13)	113.7(4)
O(16)-Al(2)-O(15)#4	109.85(10)	O(12)-P(4)-O(13)	106.9(4)
O(3)-Al(2)-O(15)#4	110.65(11)	O(1)-P(4)-O(13)	103.9(3)
O(16)-Al(2)-O(13)	107.77(11)	O(7)-Al(1)-O(10)#1	109.9(3)
O(3)-Al(2)-O(13)	109.71(10)	O(7)-Al(1)-O(4)	110.3(3)
O(15)#4-Al(2)-O(13)	107.23(10)	O(10)#1-Al(1)-O(4)	111.4(3)
O(1)#5-Al(3)-O(11)	108.65(11)	O(7)-Al(1)-O(1)	109.5(3)
O(1)#5-Al(3)-O(8)#6	110.29(11)	O(10)#1-Al(1)-O(1)	106.0(3)
O(11)-Al(3)-O(8)#6	109.91(11)	O(4)-Al(1)-O(1)	109.5(3)
O(1)#5-Al(3)-O(7)	109.25(11)	O(11)#2-Al(2)-O(13)#3	107.2(3)
O(11)-Al(3)-O(7)	110.18(11)	O(11)#2-Al(2)-O(2)#3	110.2(3)
O(8)#6-Al(3)-O(7)	108.54(12)	O(13)#3-Al(2)-O(2)#3	110.8(3)
O(4)-P(1)-O(16)	112.43(12)	O(11)#2-Al(2)-O(3)	109.8(3)
O(4)-P(1)-O(14)	111.16(13)	O(13)#3-Al(2)-O(3)	109.0(3)
O(16)-P(1)-O(14)	106.16(13)	O(2)#3-Al(2)-O(3)	109.8(3)
O(4)-P(1)-O(6)	111.55(13)	O(15)#4-Al(3)-O(9)#5	114.7(4)
O(16)-P(1)-O(6)	106.71(12)	O(15)#4-Al(3)-O(8)#6	109.7(4)
O(14)-P(1)-O(6)	108.56(14)	O(9)#5-Al(3)-O(8)#6	109.6(3)
O(12)-P(2)-O(5)	113.25(12)	O(15)#4-Al(3)-O(12)	106.4(4)
O(12)-P(2)-O(8)	108.93(12)	O(9)#5-Al(3)-O(12)	108.1(4)
O(5)-P(2)-O(8)	110.14(13)	O(8)#6-Al(3)-O(12)	108.1(3)
O(12)-P(2)-O(11)	110.77(12)	O(16)#7-Mg(1)-O(14)	151.5(3)
O(5)-P(2)-O(11)	106.66(12)	O(16)#7-Mg(1)-O(5)	105.9(3)
O(8)-P(2)-O(11)	106.90(12)	O(14)-Mg(1)-O(5)	101.9(3)
O(10)-P(3)-O(3)	112.97(12)	O(16)#7-Mg(1)-O(6)	93.2(3)

O(10)-P(3)-O(1)	110.19(13)	O(14)-Mg(1)-O(6)	88.7(3)
O(3)-P(3)-O(1)	108.04(12)	O(5)-Mg(1)-O(6)	98.6(3)
O(10)-P(3)-O(15)	111.86(13)	O(16)#7-Mg(1)-O(17)	84.9(3)
O(3)-P(3)-O(15)	106.79(12)	O(14)-Mg(1)-O(17)	85.8(3)
O(1)-P(3)-O(15)	106.70(12)	O(5)-Mg(1)-O(17)	96.7(4)
O(9)-P(4)-O(2)	112.01(13)	O(6)-Mg(1)-O(17)	164.6(4)
O(9)-P(4)-O(13)	114.15(12)		
O(2)-P(4)-O(13)	105.36(12)		
O(9)-P(4)-O(7)	113.75(13)		
O(2)-P(4)-O(7)	107.47(13)		
O(13)-P(4)-O(7)	103.32(12)		

For JU94: Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1 #2 x,-y+1/2,z-1/2 #3 -x,y+1/2,-z+3/2 #4 x,-y+1/2,z+1/2 #5 -x-1,-y,-z+1 #6 x,-y-1/2,z+1/2 #7 -x,y-1/2,-z+3/2 #8 x,-y-1/2,z-1/2 #9 -x-1,-y,-z

For JU94-400: Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2 #2 -x,y-1/2,-z-1/2 #3 x,-y-1/2,z-1/2 #4 -x+1,-y,-z+1 #5 -x+1,y-1/2,-z+1/2 #6 x,-y-1/2,z+1/2 #7 -x+1,-y,-z #8 -x+1,y+1/2,-z+1/2 #9 x,-y+1/2,z-1/2 #10 -x,y+1/2,-z-1/2 #11 -x,-y+2,-z+1

Table S4. Selected bond lengths [Å] and angles [deg] for JU95 and JU95-300.

JU95		JU95-300	
P(1)-O(2)	1.496(2)	P(1)-O(13)	1.499(3)
P(1)-O(3)	1.5287(19)	P(1)-O(2)	1.512(3)
P(1)-O(1)	1.5383(18)	P(1)-O(12)	1.514(3)
P(1)-O(4)	1.5382(19)	P(1)-O(1)	1.540(3)
P(2)-O(6)	1.483(2)	P(2)-O(7)	1.511(3)
P(2)-O(7)	1.517(2)	P(2)-O(16)	1.519(3)
P(2)-O(8)	1.521(2)	P(2)-O(5)	1.519(3)
P(2)-O(5)	1.5380(18)	P(2)-O(3)	1.533(3)
P(3)-O(11)	1.489(2)	P(3)-O(15)	1.487(3)
P(3)-O(12)	1.512(2)	P(3)-O(9)	1.521(3)
P(3)-O(10)	1.521(2)	P(3)-O(14)	1.525(3)
P(3)-O(9)	1.535(2)	P(3)-O(6)	1.551(3)
P(4)-O(16)	1.482(2)	P(4)-O(4)	1.490(3)
P(4)-O(13)	1.530(2)	P(4)-O(11)	1.529(3)
P(4)-O(14)	1.5328(18)	P(4)-O(8)	1.531(3)
P(4)-O(15)	1.537(2)	P(4)-O(10)#1	1.536(3)
Al(1)-O(12)#1	1.703(2)	P(4)-Mg(1)	3.1516(17)
Al(1)-O(13)	1.719(2)	Al(2)-O(10)	1.707(3)
Al(1)-O(7)#2	1.721(2)	Al(2)-O(12)	1.711(3)
Al(1)-O(3)	1.730(2)	Al(2)-O(6)	1.749(3)
Al(2)-O(5)	1.725(2)	Al(2)-O(3)	1.758(3)
Al(2)-O(10)#3	1.726(2)	Al(3)-O(5)	1.715(3)
Al(2)-O(15)#4	1.732(2)	Al(3)-O(9)#2	1.725(3)
Al(2)-O(1)	1.7448(19)	Al(3)-O(11)	1.725(3)
Al(3)-O(8)#5	1.718(2)	Al(3)-O(1)	1.746(3)
Al(3)-O(14)	1.726(2)	Al(1)-O(2)	1.711(3)
Al(3)-O(4)#3	1.740(2)	Al(1)-O(14)#4	1.723(3)
Al(3)-O(9)	1.745(2)	Al(1)-O(8)#4	1.734(3)
Mg(8)-O(16)	1.992(2)	Al(1)-O(16)#5	1.734(3)
Mg(8)-O(11)#6	2.039(2)	Mg(1)-O(15)#3	1.902(3)
Mg(8)-O(6)#7	2.051(2)	Mg(1)-O(4)	1.917(3)
Mg(8)-O(2)	2.068(2)	Mg(1)-O(13)#3	1.928(3)
Mg(8)-O(17)	2.126(2)	Mg(1)-O(7)	1.994(3)
Mg(8)-O(18)	2.199(3)	N(1)-C(1)	1.496(7)
N(1)-C(2)	1.489(5)	N(1)-C(2)	1.502(7)
N(1)-C(1)	1.508(4)	C(1)-C(2)#11	1.520(7)
C(2)-C(1)#13	1.514(6)	C(2)-C(1)#11	1.520(7)
C(1)-C(2)#13	1.514(6)		
O(2)-P(1)-O(3)	111.51(12)	O(13)-P(1)-O(2)	111.67(19)
O(2)-P(1)-O(1)	110.56(11)	O(13)-P(1)-O(12)	111.33(18)
O(3)-P(1)-O(1)	105.23(11)	O(2)-P(1)-O(12)	108.3(2)

O(2)-P(1)-O(4)	113.28(12)	O(13)-P(1)-O(1)	110.61(19)
O(3)-P(1)-O(4)	108.19(12)	O(2)-P(1)-O(1)	105.71(18)
O(1)-P(1)-O(4)	107.67(11)	O(12)-P(1)-O(1)	109.01(18)
O(6)-P(2)-O(7)	112.06(16)	O(7)-P(2)-O(16)	111.37(19)
O(6)-P(2)-O(8)	110.66(16)	O(7)-P(2)-O(5)	111.25(18)
O(7)-P(2)-O(8)	108.17(18)	O(16)-P(2)-O(5)	108.68(19)
O(6)-P(2)-O(5)	112.59(12)	O(7)-P(2)-O(3)	109.42(17)
O(7)-P(2)-O(5)	107.04(12)	O(16)-P(2)-O(3)	106.46(16)
O(8)-P(2)-O(5)	106.01(13)	O(5)-P(2)-O(3)	109.53(16)
O(11)-P(3)-O(12)	110.51(17)	O(10)-Al(2)-O(12)	110.46(17)
O(11)-P(3)-O(10)	112.52(13)	O(10)-Al(2)-O(6)	110.53(16)
O(12)-P(3)-O(10)	108.78(14)	O(12)-Al(2)-O(6)	115.58(17)
O(11)-P(3)-O(9)	110.29(12)	O(10)-Al(2)-O(3)	108.24(15)
O(12)-P(3)-O(9)	106.11(15)	O(12)-Al(2)-O(3)	108.64(15)
O(10)-P(3)-O(9)	108.39(12)	O(6)-Al(2)-O(3)	102.90(15)
O(16)-P(4)-O(13)	112.93(13)	O(15)-P(3)-O(9)	111.81(18)
O(16)-P(4)-O(14)	109.87(12)	O(15)-P(3)-O(14)	112.2(2)
O(13)-P(4)-O(14)	106.67(11)	O(9)-P(3)-O(14)	107.49(17)
O(16)-P(4)-O(15)	113.26(14)	O(15)-P(3)-O(6)	110.86(18)
O(13)-P(4)-O(15)	106.38(12)	O(9)-P(3)-O(6)	107.28(17)
O(14)-P(4)-O(15)	107.36(12)	O(14)-P(3)-O(6)	106.88(18)
O(12)#1-Al(1)-O(13)	108.47(12)	O(4)-P(4)-O(11)	111.74(19)
O(12)#1-Al(1)-O(7)#2	110.58(16)	O(4)-P(4)-O(8)	111.32(18)
O(13)-Al(1)-O(7)#2	108.58(11)	O(11)-P(4)-O(8)	107.40(16)
O(12)#1-Al(1)-O(3)	106.74(14)	O(4)-P(4)-O(10)#1	112.35(19)
O(13)-Al(1)-O(3)	112.04(10)	O(11)-P(4)-O(10)#1	107.28(18)
O(7)#2-Al(1)-O(3)	110.42(13)	O(8)-P(4)-O(10)#1	106.45(17)
O(5)-Al(2)-O(10)#3	108.69(11)	O(4)-P(4)-Mg(1)	25.45(13)
O(5)-Al(2)-O(15)#4	111.46(11)	O(11)-P(4)-Mg(1)	92.35(13)
O(10)#3-Al(2)-O(15)#4	115.66(12)	O(8)-P(4)-Mg(1)	103.96(12)
O(5)-Al(2)-O(1)	106.42(9)	O(10)#1-P(4)-Mg(1)	136.38(13)
O(10)#3-Al(2)-O(1)	108.38(10)	O(5)-Al(3)-O(9)#2	107.47(16)
O(15)#4-Al(2)-O(1)	105.77(11)	O(5)-Al(3)-O(11)	111.99(17)
O(8)#5-Al(3)-O(14)	112.19(12)	O(9)#2-Al(3)-O(11)	110.18(14)
O(8)#5-Al(3)-O(4)#3	115.71(12)	O(5)-Al(3)-O(1)	110.48(15)
O(14)-Al(3)-O(4)#3	105.55(10)	O(9)#2-Al(3)-O(1)	110.69(16)
O(8)#5-Al(3)-O(9)	105.09(14)	O(11)-Al(3)-O(1)	106.07(16)
O(14)-Al(3)-O(9)	108.04(10)	O(15)#3-Mg(1)-O(4)	109.36(16)
O(4)#3-Al(3)-O(9)	110.10(10)	O(15)#3-Mg(1)-O(13)#3	110.47(15)
O(16)-Mg(8)-O(11)#6	96.00(11)	O(4)-Mg(1)-O(13)#3	124.33(16)
O(16)-Mg(8)-O(6)#7	92.68(11)	O(15)#3-Mg(1)-O(7)	108.03(16)
O(11)#6-Mg(8)-O(6)#7	170.00(11)	O(4)-Mg(1)-O(7)	105.19(15)
O(16)-Mg(8)-O(2)	96.59(10)	O(13)#3-Mg(1)-O(7)	97.66(15)
O(11)#6-Mg(8)-O(2)	89.04(9)	O(15)#3-Mg(1)-P(4)	105.19(11)

O(6)#7-Mg(8)-O(2)	94.91(9)	O(4)-Mg(1)-P(4)	19.51(10)
O(16)-Mg(8)-O(17)	90.08(10)	O(13)#3-Mg(1)-P(4)	139.40(11)
O(11)#6-Mg(8)-O(17)	90.01(9)	O(7)-Mg(1)-P(4)	89.03(11)
O(6)#7-Mg(8)-O(17)	85.01(9)	O(2)-Al(1)-O(14)#4	109.22(17)
O(2)-Mg(8)-O(17)	173.32(10)	O(2)-Al(1)-O(8)#4	110.71(16)
O(16)-Mg(8)-O(18)	175.92(10)	O(14)#4-Al(1)-O(8)#4	106.78(15)
O(11)#6-Mg(8)-O(18)	87.53(11)	O(2)-Al(1)-O(16)#5	108.17(17)
O(6)#7-Mg(8)-O(18)	83.63(11)	O(14)#4-Al(1)-O(16)#5	113.48(16)
O(2)-Mg(8)-O(18)	85.48(9)	O(8)#4-Al(1)-O(16)#5	108.49(16)
O(17)-Mg(8)-O(18)	87.88(10)		

For JU95: Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z+1/2 #2 -x,-y+1,-z+1 #3 -x,-y+1,-z #4 -x+1/2,y+1/2,-z+1/2 #5 -x-1/2,y-1/2,-z+1/2 #6 x+1/2,-y+1/2,z+1/2 #7 x+1/2,-y+3/2,z-1/2 #8 x-1/2,-y+3/2,z+1/2 #9 -x+1/2,y-1/2,-z+1/2 #10 x-1/2,-y+1/2,z-1/2 #11 x+1/2,-y+1/2,z-1/2 #12 -x-1/2,y+1/2,-z+1/2 #13 -x,-y,-z

For JU95-300: Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z+1/2 #2 x+1/2,-y+1/2,z+1/2 #3 -x-1/2,y+1/2,-z+3/2 #4 x+1,y,z #5 -x+1/2,y-1/2,-z+3/2 #6 x-1,y,z #7 x-1/2,-y+1/2,z-1/2 #8 x+1/2,-y+1/2,z-1/2 #9 -x-1/2,y-1/2,-z+3/2 #10 -x+1/2,y+1/2,-z+3/2 #11 -x-1,-y+1,-z+1

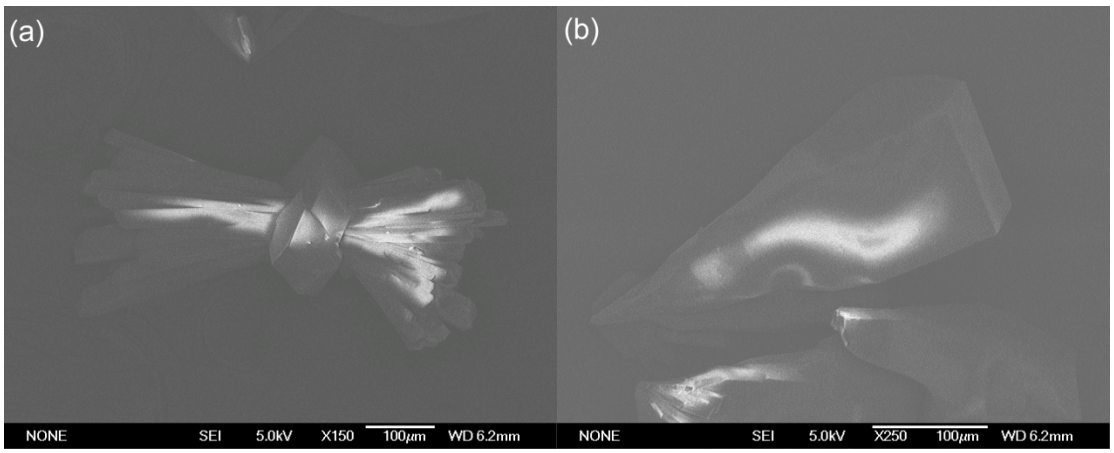
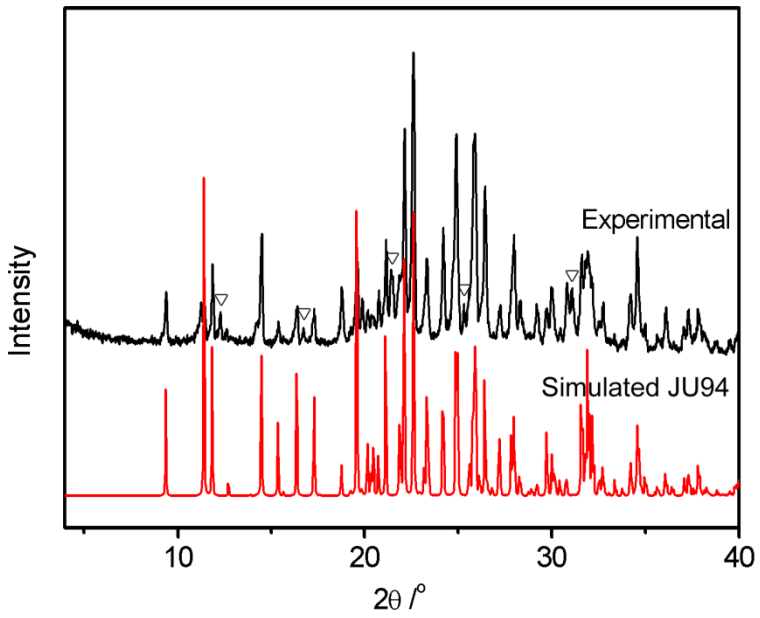
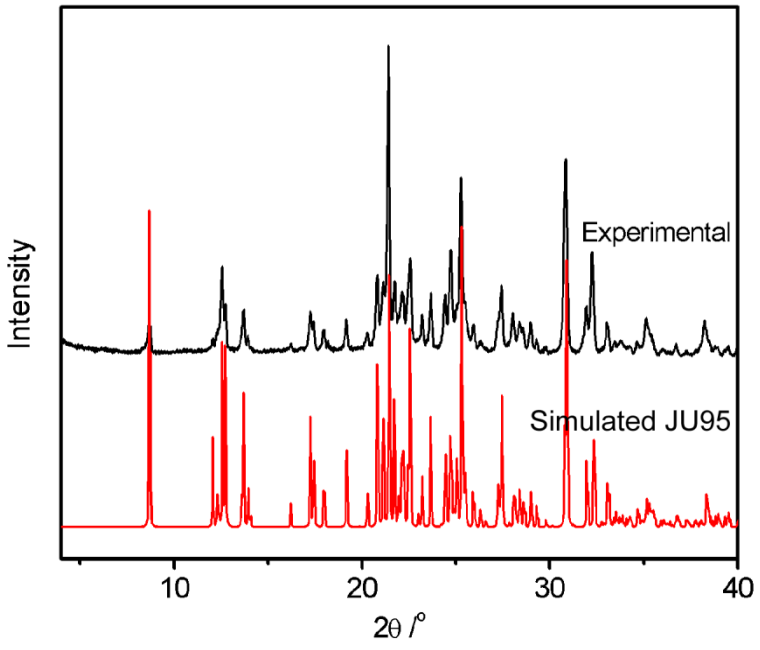


Figure S1. SEM images of (a) JU94 (the thin rod-like crystal) and the unknown phase (the block crystal in the center) and (b) JU95 (the rod-like crystal).

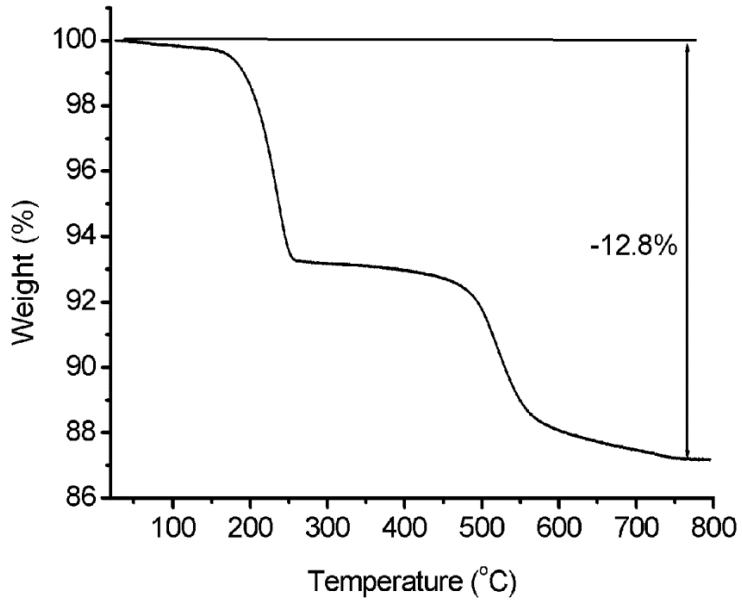


(a)

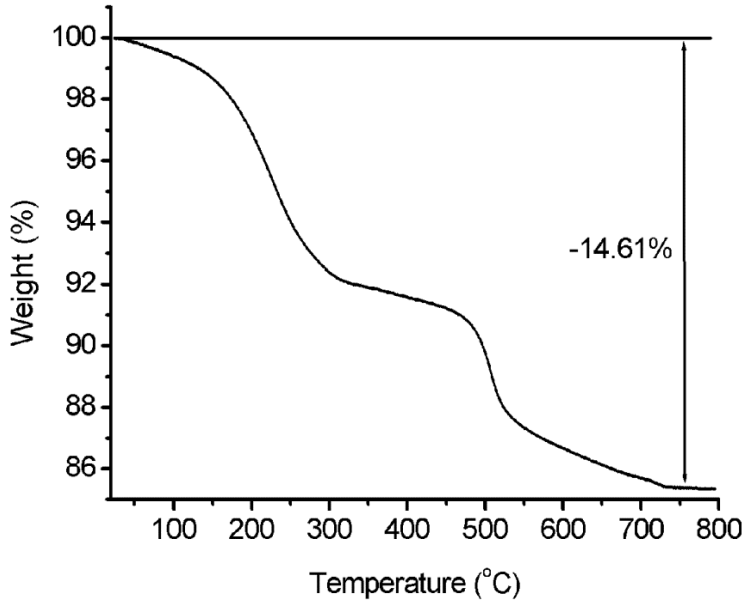


(b)

Figure S2. Experimental and simulated PXRD patterns of (a) JU94 (peaks of impurity are marked by triangle) and (b) JU95.



(a)



(b)

Figure S3. TG curves of (a) JU94 and (b) JU95.

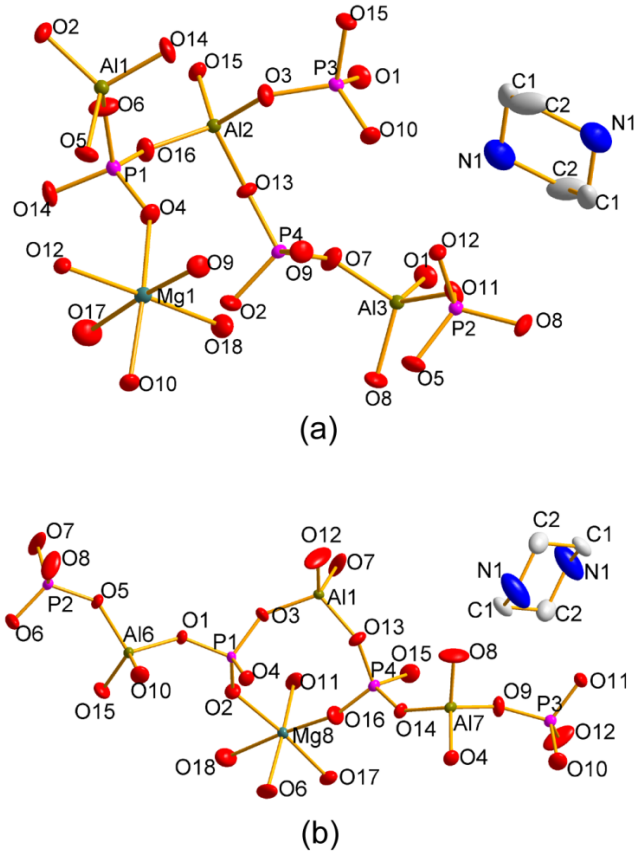


Figure S4. Thermal ellipsoids of (a) JU94 and (b) JU95 given at 50% probability, showing the atomic labeling scheme.

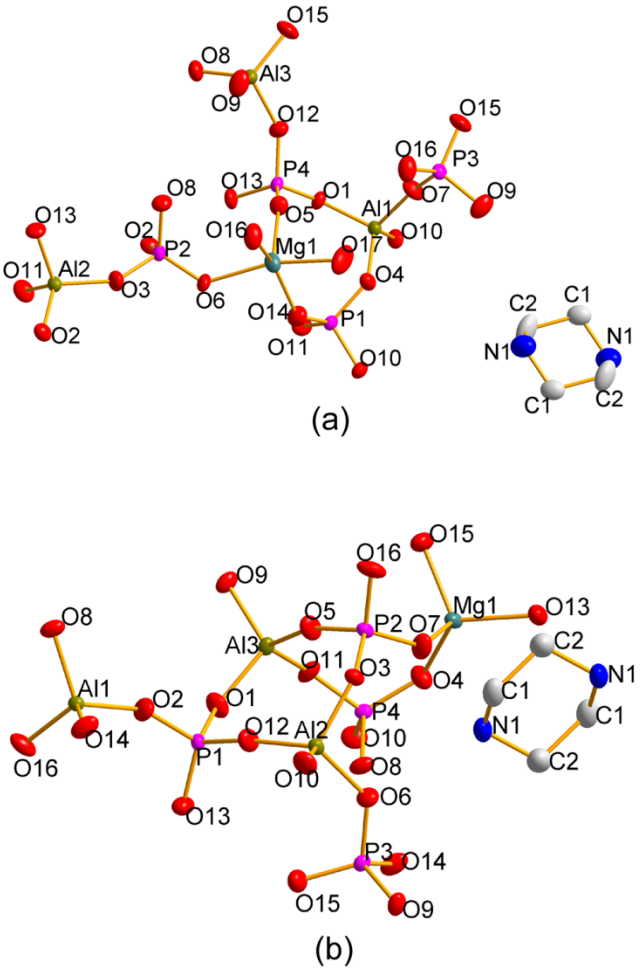


Figure S5. Thermal ellipsoids of (a) JU94-400 and (b) JU95-300 given at 50% probability, showing the atomic labelling scheme.