Electronic supplementary information (ESI)

Concise template syntheses of gallium phosphatesdriven by *in situ* direct alkylation of aliphatic and aromatic precursors by methanols

Guo-Ming Wang*, Jin-Hua Li, Li Wei, Xiao Zhang and Zhen-Zhen Bao

Teachers College,College of Chemical Science and Engineering, Collaborative Innovation Center for Marine BiomassFiber Materials and Textiles, Qingdao University, Shandong 266071, P. R. China

*Corresponding author. E-mail: gmwang_pub@163.com. Fax: +86-532-85956024

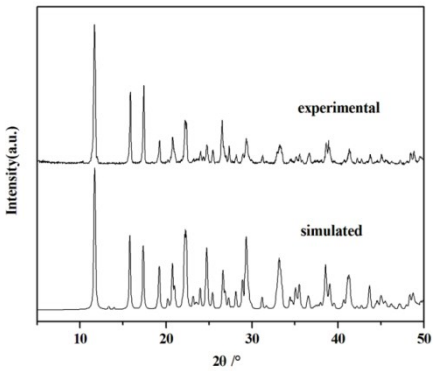

Fig.S1 The PXRD patters of **1**.

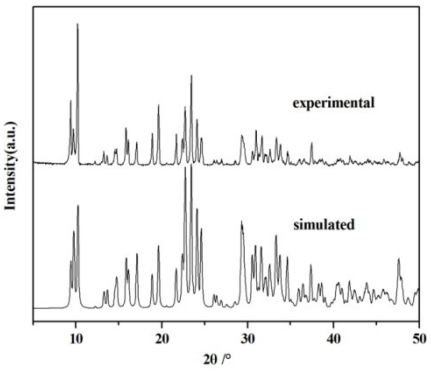

Fig.S2 The PXRD patters of **2**.

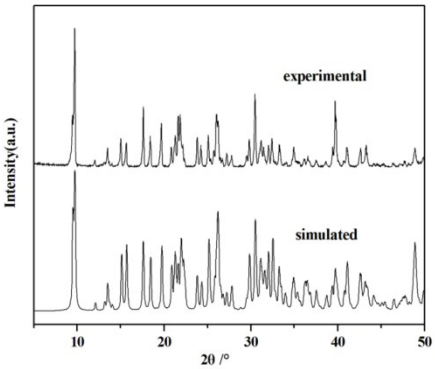

Fig.S3 The PXRD patters of **3**.

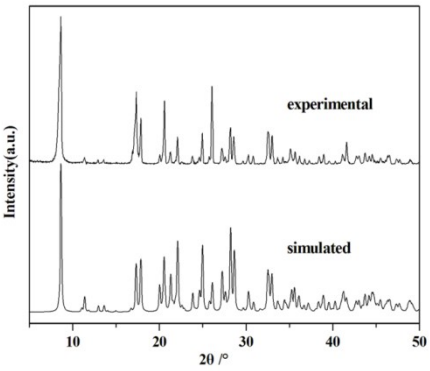

Fig.S4 The PXRD patters of **4**.

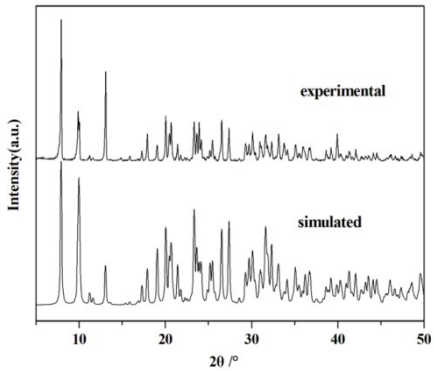

Fig.S5 The PXRD patters of **5**.

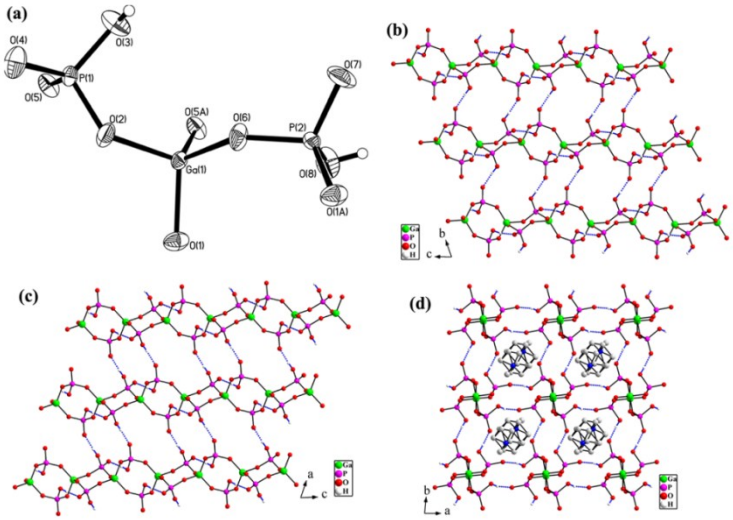

Fig.S6 (a) View of the coordination of the gallium and phosphorus atoms in **1**, showing the atom-labeling schemeand 50% thermal ellipsoids;(b,c,d)Views of hydrogen-bonded network made up of the adjacent chains by H-bonding.

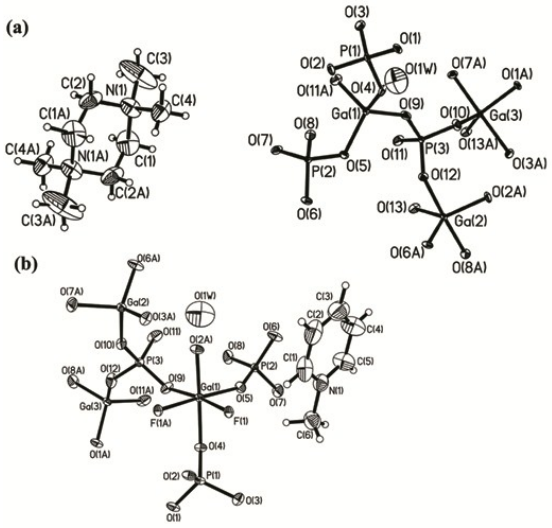

Fig.S7 ORTEPplots of themolecular structures of **2** (a)and **3**(b), drawn at the 50% probability level respectively.

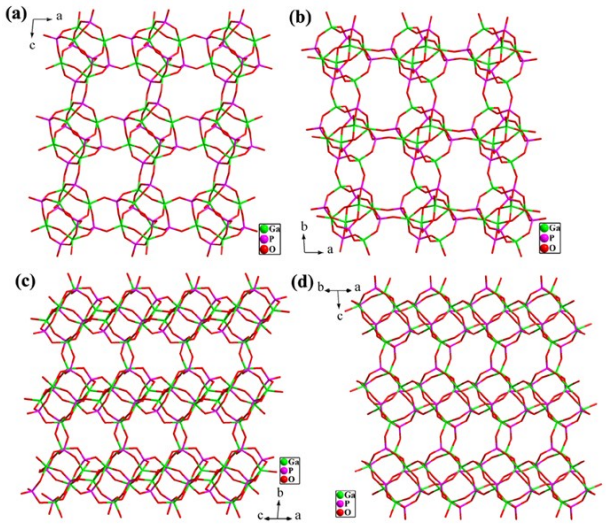

Fig.S8 Perspective view of the 3D structure made up of Ga_6P_6SBUs, showing regular 8-ring channels along the [010](a), [001] (b), [101](c) and [110] (d)directions in compound **2**.

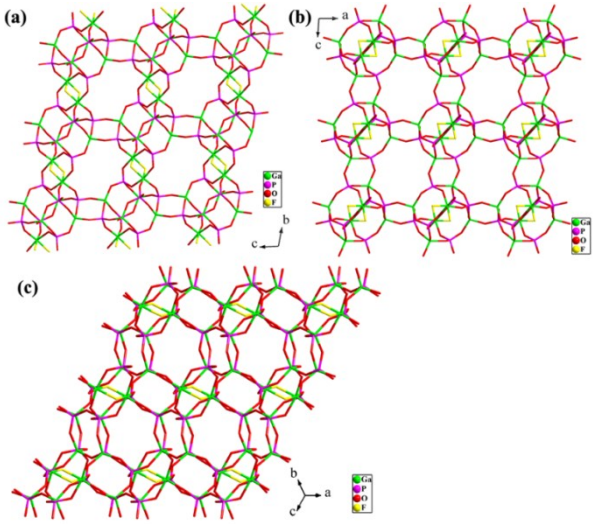

Fig.S9 Perspective view of the 3D structure of **3**, showing regular 8-ring channels along the [100](a), [010](b)and [111] (c)directions.

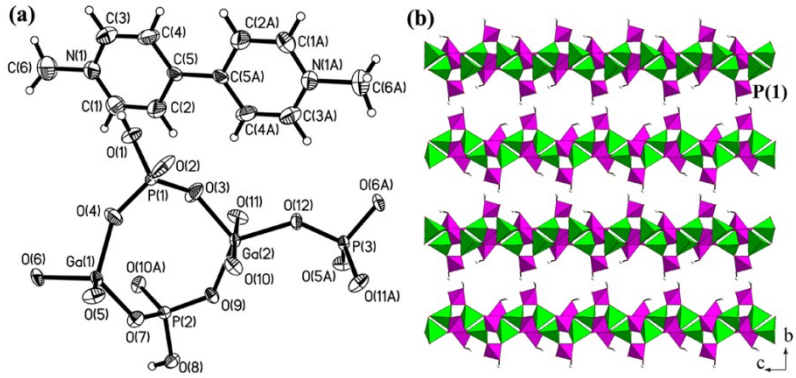

Fig.S10(a) ORTEP plot of themolecular structure of **4**, drawnat the 50% probability level;(b)Polyhedral view ofthe packing of the sheets along the [010] direction, with terminalP=O and P-OH groups pointing into the interlayerspace.

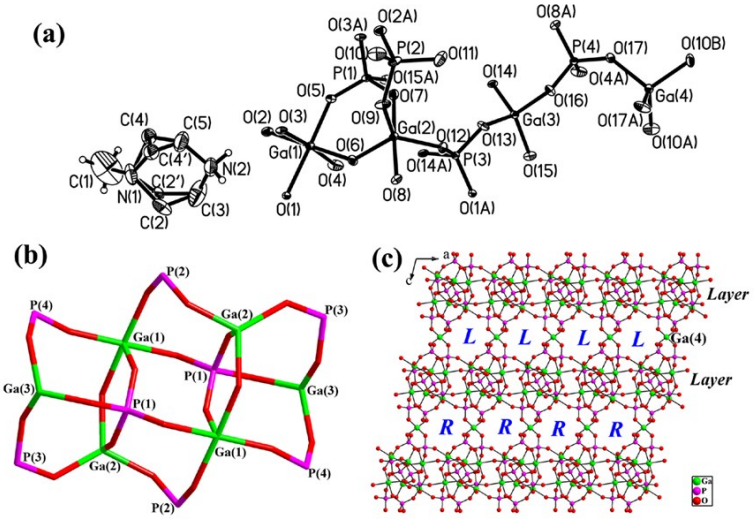

Fig.S11(a) ORTEPplot of themolecular structure of **5**, drawnat the 50% probability level;(b)The structure of the Ga_6P_8 cluster in compound**5**;(c)The 2D sheets are stacked and pillared by Ga(4)O_4nodes to form 3D structure withhelical channels along the [010] direction.

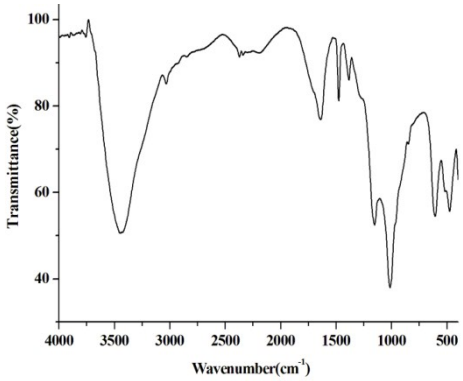

Fig. S12 The IR spectrum of **1**.

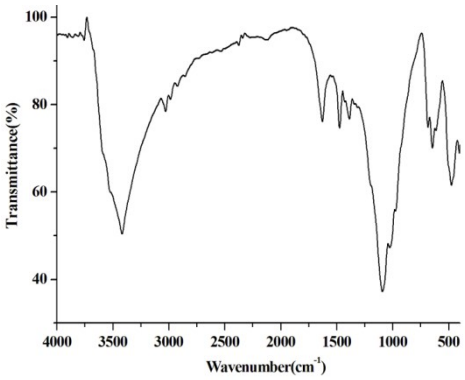

Fig. S13 The IR spectrum of **2**.

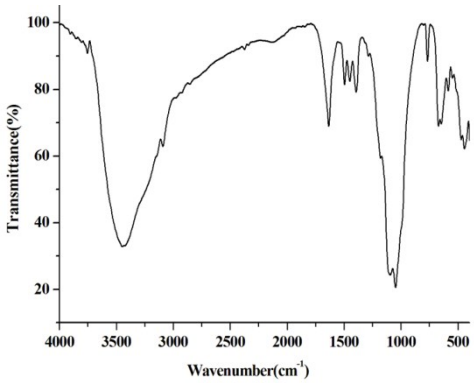

Fig. S14 The IR spectrum of **3**.

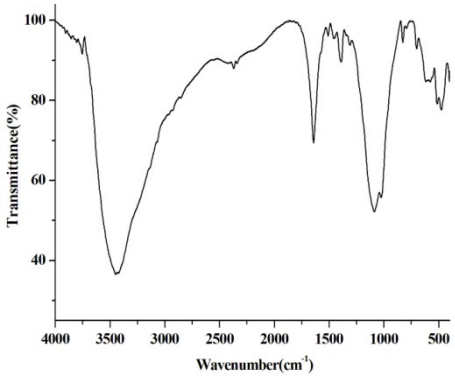

Fig. S15 The IR spectrum of **4**.

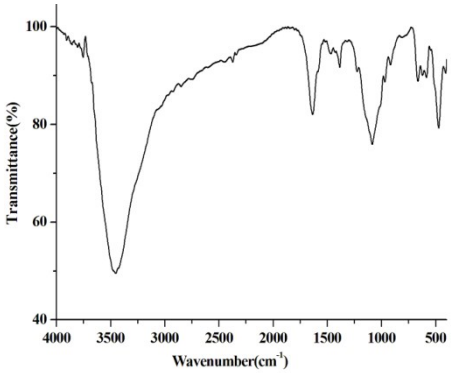

Fig. S16 The IR spectrum of **5**.

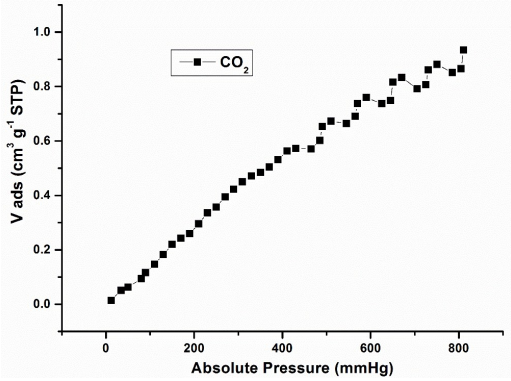

Fig. S17 CO_2 adsorption at 273K for**3**.

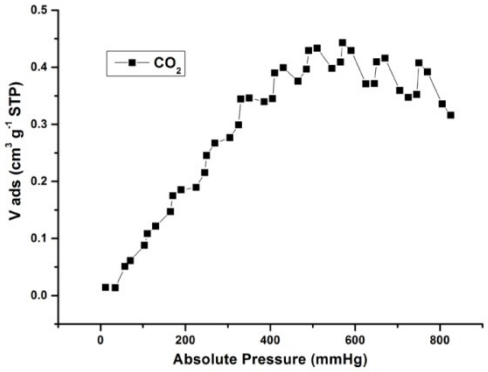

Fig. S18 CO_2 adsorption at 273K for **5**.

Table S1 Details of hydrogen bonds for **1-5**.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
	Compound **1**			
O(3)–H(3A) ···O(127)	0.82	1.70	2.496(4)	163.9
O(8)–H(8A) ···O(4)	0.82	1.71	2.530(5)	175.1
	Compound **2**			
C(1) –H(1A) ···O(12)	0.97	2.40	3.351(5)	166
C(2) –H(2A) ···O(7)	0.97	2.40	3.361(5)	169
C(4) –H(4C) ···O(5)	0.96	2.57	3.519(8)	172
	Compound **3**			
C(1) –H(1A) ···F(1)	0.93	2.51	3.128(2)	124
C(5) –H(5A) ···O(3)	0.93	2.43	3.273(5)	151
C(6) –H(6A) ···O(3)	0.96	2.51	3.386(5)	152
C(6) –H(6B) ··· F(1)	0.96	2.39	3.158(1)	136
	Compound **4**			
O(1)–H(1A) ···O(2)	0.82	1.72	2.521(4)	165.1
O(8)–H(8A) ···O(2)	0.82	1.71	2.527(4)	171.4
C(1) –H(1B) ···O(8)	0.93	2.41	3.149(3)	136
C(3) –H(3A) ···O(5)	0.93	2.58	3.406(5)	149
C(4) –H(4A) ···O(10)	0.93	2.42	3.145(2)	135
C(6) –H(6A) ···O(4)	0.93	2.58	3.209(8)	124
	Compound **5**			
N(2)–H(2A) ···O(3)	0.90	2.60	3.066(7)	112.7
N(2)–H(2A) ···O(2)	0.90	1.97	2.856(7)	167.8

Table S2 Selected bond lengths (Å) and bond angels (°) for **1-5**

Compound **1**			
Ga(1)-O(6)	1.814(3) [0.797]	P(1)-O(3)	1.555(3)[1.182]
Ga(1)-O(2)	1.814(3)[0.797]	Σ(P(1)-O)	**5.032**
Ga(1)-O(5)#1	1.814(3)[0.797]	P(2)-O(7)	1.486(3)[1.425]
Ga(1)-O(1)	1.822(3)[0.779]	P(2)-O(6)	1.537(3)[1.241]
Σ(Ga(1)-O)	**3.170**	P(2)-O(1)#2	1.542(3)[1.225]
P(1)-O(4)	1.482(3) [1.440]	P(2)-O(8)	1.560(3)[1.166]
P(1)-O(5)	1.547(3) [1.208]	Σ(P(2)-O)	**5.057**
P(1)-O(2)	1.549(3)[1.202]		
O(6)-Ga(1)-O(2)	105.72(14)	O(4)-P(1)-O(3)	113.8(2)
O(6)-Ga(1)-O(5)#1	108.10(13)	O(5)-P(1)-O(3)	103.79(17)
O(2)-Ga(1)-O(5)#1	113.35(13)	O(2)-P(1)-O(3)	108.30(18)
O(6)-Ga(1)-O(1)	111.02(13)	O(7)-P(2)-O(6)	111.05(19)
O(2)-Ga(1)-O(1)	107.70(14)	O(7)-P(2)-O(1)#2	110.34(18)
O(5)#1-Ga(1)-O(1)	110.87(14)	O(6)-P(2)-O(1)#2	107.44(17)
O(4)-P(1)-O(5)	112.25(18)	O(7)-P(2)-O(8)	113.38(19)
O(4)-P(1)-O(2)	110.29(19)	O(6)-P(2)-O(8)	105.86(17)
O(5)-P(1)-O(2)	108.00(18)	O(1)#2-P(2)-O(8)	108.51(18)
Compound **2**			
Ga(1)-O(4)	1.809(3)[0.808]	Σ(Ga(3)-O)	**3.069**
Ga(1)-O(9)	1.826(3)[0.771]	P(1)-O(1)	1.518(3)[1.306]
Ga(1)-O(5)	1.829(3)[0.765]	P(1)-O(2)	1.525(4)[1.282]
Ga(1)-O(11)#1	1.839(4)[0.745]	P(1)-O(3)	1.528(4)[1.271]
Σ(Ga(1)-O)	**3.089**	P(1)-O(4)	1.558(3)[1.172]
Ga(2)-O(6)#2	1.864(3)[0.696]	Σ(P(1)-O)	**5.031**
Ga(2)-O(2)#3	1.867(3)[0.691]	P(2)-O(7)	1.508(4) [1.342]
Ga(2)-O(13)	1.906(3)[0.621]	P(2)-O(8)	1.521(3) [1.296]
Ga(2)-O(8)#3	1.919(3)[0.600]	P(2)-O(6)	1.542(3) [1.224]
Ga(2)-O(12)	1.977(3)[0.513]	P(2)-O(5)	1.567(4) [1.144]
Σ(Ga(2)-O)	**3.121**	Σ(P(2)-O)	**5.006**
Ga(3)-O(1)#4	1.854(3) [0.715]	P(3)-O(12)	1.520(3) [1.299]
Ga(3)-O(10)	1.865(3) [0.694]	P(3)-O(10)	1.523(4) [1.289]
Ga(3)-O(13)#5	1.923(3) [0.594]	P(3)-O(9)	1.534(3) [1.251]
Ga(3)-O(7)#1	1.953(3) [0.547]	P(3)-O(11)	1.556(4) [1.179]
Ga(3)-O(3)#3	1.973(3) [0.519]	Σ(P(3)-O)	**5.018**
O(4)-Ga(1)-O(9)	104.86(16)	O(1)#4-Ga(3)-O(3)#3	91.02(15)

O(4)-Ga(1)-O(5)	116.73(16)	O(10)-Ga(3)-O(3)#3	93.86(15)
O(9)-Ga(1)-O(5)	108.88(15)	O(13)#5-Ga(3)-O(3)#3	82.90(14)
O(4)-Ga(1)-O(11)#1	108.27(15)	O(7)#1-Ga(3)-O(3)#3	171.32(15)
O(9)-Ga(1)-O(11)#1	108.61(17)	O(1)-P(1)-O(2)	105.9(2)
O(5)-Ga(1)-O(11)#1	109.20(17)	O(1)-P(1)-O(3)	113.4(2)
O(6)#2-Ga(2)-O(2)#3	116.37(16)	O(2)-P(1)-O(3)	112.2(2)
O(6)#2-Ga(2)-O(13)	118.22(16)	O(1)-P(1)-O(4)	107.0(2)
O(2)#3-Ga(2)-O(13)	125.10(16)	O(2)-P(1)-O(4)	110.6(2)
O(6)#2-Ga(2)-O(8)#3	94.84(14)	O(3)-P(1)-O(4)	107.56(19)
O(2)#3-Ga(2)-O(8)#3	88.71(15)	O(7)-P(2)-O(8)	113.2(2)
O(13)-Ga(2)-O(8)#3	92.15(15)	O(7)-P(2)-O(6)	109.7(2)
O(6)#2-Ga(2)-O(12)	86.72(14)	O(8)-P(2)-O(6)	112.35(19)
O(2)#3-Ga(2)-O(12)	88.60(15)	O(7)-P(2)-O(5)	110.1(2)
O(13)-Ga(2)-O(12)	89.06(15)	O(8)-P(2)-O(5)	106.9(2)
O(8)#3-Ga(2)-O(12)	177.28(14)	O(6)-P(2)-O(5)	104.06(19)
O(1)#4-Ga(3)-O(10)	115.42(15)	O(12)-P(3)-O(10)	112.5(2)
O(1)#4-Ga(3)-O(13)#5	124.61(16)	O(12)-P(3)-O(9)	110.32(19)
O(10)-Ga(3)-O(13)#5	119.90(16)	O(10)-P(3)-O(9)	105.98(19)
O(1)#4-Ga(3)-O(7)#1	88.92(15)	O(12)-P(3)-O(11)	106.6(2)
O(10)-Ga(3)-O(7)#1	94.00(16)	O(10)-P(3)-O(11)	110.5(2)
O(13)#5-Ga(3)-O(7)#1	89.99(15)	O(9)-P(3)-O(11)	111.0(2)

Compound **3**

Ga(1)-O(5)	1.893(3)[0.644]	Σ(Ga(3)-O)	**3.238**
Ga(1)-O(9)	1.907(3)[0.619]	P(1)-O(4)	1.514(3)[1.321]
Ga(1)-O(4)	1.934(3) [0.576]	P(1)-O(2)	1.527(3)[1.275]
Ga(1)-O(2)#1	1.946(3) [0.558]	P(1)-O(1)	1.548(3)[1.205]
Ga(1)-F(1)	1.973(2) [0.385]	P(1)-O(3)	1.555(3)[1.182]
Ga(1)-F(1)#1	1.983(2) [0.375]	Σ(P(1)-O)	**4.983**
Σ(Ga(1)-O/F)	**3.157**	P(2)-O(5)	1.498(3)[1.379]
Ga(2)-O(10)	1.804(3) [0.818]	P(2)-O(8)	1.524(3) [1.285]
Ga(2)-O(7)#2	1.809(3) [0.808]	P(2)-O(7)	1.530(3) [1.265]
Ga(2)-O(6)#3	1.816(3) [0.793]	P(2)-O(6)	1.540(3) [1.231]
Ga(2)-O(3)#1	1.818(3) [0.788]	Σ(P(2)-O)	**5.160**
Σ(Ga(2)-O)	**3.207**	P(3)-O(9)	1.505(3) [1.353]
Ga(3)-O(8)#4	1.800(3) [0.827]	P(3)-O(10)	1.524(3) [1.285]
Ga(3)-O(11)#4	1.804(3) [0.818]	P(3)-O(12)	1.527(3) [1.275]
Ga(3)-O(1)#5	1.810(3) [0.805]	P(3)-O(11)	1.530(3) [1.265]
Ga(3)-O(12)	1.818(3) [0.788]	Σ(P(3)-O)	**5.178**

O(5)-Ga(1)-O(9)	97.59(13)	O(11)#4-Ga(3)-O(1)#5	110.33(14)
O(5)-Ga(1)-O(4)	94.11(12)	O(8)#4-Ga(3)-O(12)	101.65(15)
O(9)-Ga(1)-O(4)	92.99(12)	O(11)#4-Ga(3)-O(12)	110.35(16)
O(5)-Ga(1)-O(2)#1	93.88(12)	O(1)#5-Ga(3)-O(12)	103.94(15)
O(9)-Ga(1)-O(2)#1	95.95(12)	O(4)-P(1)-O(2)	116.82(16)
O(4)-Ga(1)-O(2)#1	167.11(12)	O(4)-P(1)-O(1)	106.18(16)
O(5)-Ga(1)-F(1)	91.73(11)	O(2)-P(1)-O(1)	110.05(17)
O(9)-Ga(1)-F(1)	170.53(11)	O(4)-P(1)-O(3)	108.91(16)
O(4)-Ga(1)-F(1)	84.64(11)	O(2)-P(1)-O(3)	107.64(16)
O(2)#1-Ga(1)-F(1)	85.03(11)	O(1)-P(1)-O(3)	106.84(17)
O(5)-Ga(1)-F(1)#1	171.94(11)	O(5)-P(2)-O(8)	113.28(17)
O(9)-Ga(1)-F(1)#1	90.47(11)	O(5)-P(2)-O(7)	107.87(18)
O(4)-Ga(1)-F(1)#1	85.64(11)	O(8)-P(2)-O(7)	106.53(19)
O(2)#1-Ga(1)-F(1)#1	85.03(11)	O(5)-P(2)-O(6)	109.71(17)
F(1)-Ga(1)-F(1)#1	80.22(10)	O(8)-P(2)-O(6)	110.10(18)
O(10)-Ga(2)-O(7)#2	101.03(13)	O(7)-P(2)-O(6)	109.22(18)
O(10)-Ga(2)-O(6)#3	112.99(14)	O(9)-P(3)-O(10)	113.83(17)
O(7)#2-Ga(2)-O(6)#3	109.81(15)	O(9)-P(3)-O(12)	109.84(18)
O(10)-Ga(2)-O(3)#1	113.75(13)	O(10)-P(3)-O(12)	104.45(17)
O(7)#2-Ga(2)-O(3)#1	104.90(14)	O(9)-P(3)-O(11)	110.01(18)
O(6)#3-Ga(2)-O(3)#1	113.25(13)	O(10)-P(3)-O(11)	109.18(18)
O(8)#4-Ga(3)-O(11)#4	118.21(15)	O(12)-P(3)-O(11)	109.4(2)
O(8)#4-Ga(3)-O(1)#5	111.11(14)		

Compound **4**

Ga(1)-O(4)	1.791(3)[0.848]	P(1)-O(4)	1.510(3) [1.335]
Ga(1)-O(5)	1.809(3)[0.807]	P(1)-O(1)	1.545(3) [1.214]
Ga(1)-O(11)#1	1.809(3)[0.807]	Σ(P(1)-O)	**5.337**
Ga(1)-O(12)#2	1.814(3)[0.796]	P(2)-O(6)	1.499(3) [1.375]
Σ(Ga(1)-O)	**3.258**	P(2)-O(7)	1.512(3) [1.328]
Ga(2)-O(3)	1.835(3) [0.753]	P(2)-O(5)	1.531(3) [1.261]
Ga(2)-O(9)	1.856(3) [0.711]	P(2)-O(8)	1.556(3) [1.179]
Ga(2)-O(7)	1.857(3) [0.709]	Σ(P(2)-O)	**5.143**
Ga(2)-O(10)#3	1.939(3) [0.568]	P(3)-O(10)	1.495(3) [1.390]
Ga(2)-O(6)#4	1.951(3) [0.550]	P(3)-O(9)	1.507(3) [1.346]
Σ(Ga(2)-O)	**3.291**	P(3)-O(12)	1.532(3) [1.258]
P(1)-O(2)	1.494(3) [1.394]	P(3)-O(11)	1.536(3) [1.244]
P(1)-O(3)	1.494(3) [1.394]	Σ(P(3)-O)	**5.238**
O(4)-Ga(1)-O(5)	115.02(15)	O(2)-P(1)-O(4)	111.2(2)

O(4)-Ga(1)-O(11)#1	109.02(15)	O(3)-P(1)-O(4)	111.0(2)
O(5)-Ga(1)-O(11)#1	107.92(13)	O(2)-P(1)-O(1)	110.40(18)
O(4)-Ga(1)-O(12)#2	100.93(14)	O(3)-P(1)-O(1)	105.44(17)
O(5)-Ga(1)-O(12)#2	113.54(14)	O(4)-P(1)-O(1)	105.66(18)
O(11)#1-Ga(1)-O(12)#2	110.23(14)	O(6)-P(2)-O(7)	115.64(16)
O(3)-Ga(2)-O(9)	111.64(14)	O(6)-P(2)-O(5)	108.66(17)
O(3)-Ga(2)-O(7)	118.87(14)	O(7)-P(2)-O(5)	110.42(17)
O(9)-Ga(2)-O(7)	129.40(12)	O(6)-P(2)-O(8)	111.41(17)
O(3)-Ga(2)-O(10)#3	87.55(13)	O(7)-P(2)-O(8)	104.40(16)
O(9)-Ga(2)-O(10)#3	87.56(13)	O(5)-P(2)-O(8)	105.84(17)
O(7)-Ga(2)-O(10)#3	91.54(12)	O(10)-P(3)-O(9)	115.04(17)
O(3)-Ga(2)-O(6)#4	93.52(13)	O(10)-P(3)-O(12)	111.06(17)
O(9)-Ga(2)-O(6)#4	91.12(12)	O(9)-P(3)-O(12)	105.36(17)
O(7)-Ga(2)-O(6)#4	88.81(12)	O(10)-P(3)-O(11)	105.51(17)
O(10)#3-Ga(2)-O(6)#4	178.54(13)	O(9)-P(3)-O(11)	109.96(17)
O(2)-P(1)-O(3)	112.77(19)	O(12)-P(3)-O(11)	109.92(17)
		Compound **5**	
Ga(1)-O(4)	1.925(4)[0.590]	Σ(Ga(4)-O)	**3.224**
Ga(1)-O(5)	1.927(4)[0.587]	P(1)-O(5)	1.516(4) [1.313]
Ga(1)-O(6)	1.967(4)[0.527]	P(1)-O(7)	1.521(4) [1.296]
Ga(1)-O(3)	1.982(4)[0.506]	P(1)-O(3)#4	1.528(4) [1.272]
Ga(1)-O(2)	1.997(4)[0.486]	P(1)-O(15)#5	1.582(4) [1.099]
Ga(1)-O(1)	2.003(3)[0.478]	Σ(P(1)-O)	**4.980**
Σ(Ga(1)-O)	**3.174**	P(2)-O(2)#4	1.517(4) [1.310]
Ga(2)-O(6)	1.855(4) [0.713]	P(2)-O(11)	1.541(4) [1.228]
Ga(2)-O(9)	1.874(4) [0.677]	P(2)-O(9)	1.542(4) [1.225]
Ga(2)-O(12)	1.880(4) [0.666]	P(2)-O(10)	1.553(4) [1.189]
Ga(2)-O(7)	1.903(4) [0.626]	Σ(P(2)-O)	**4.952**
Ga(2)-O(8)	1.967(4) [0.527]	P(3)-O(1)#6	1.518(4) [1.306]
Σ(Ga(2)-O)	**3.209**	P(3)-O(12)	1.519(4) [1.303]
Ga(3)-O(13)	1.819(4) [0.786]	P(3)-O(13)	1.531(4) [1.261]
Ga(3)-O(15)	1.832(4) [0.759]	P(3)-O(14)#5	1.557(4) [1.176]
Ga(3)-O(16)	1.841(4) [0.741]	Σ(P(3)-O)	**5.046**
Ga(3)-O(14)	1.842(4) [0.738]	P(4)-O(4)#5	1.487(4) [1.420]
Σ(Ga(3)-O)	**3.024**	P(4)-O(8)#7	1.521(4) [1.296]
Ga(4)-O(10)#1	1.809(4) [0.807]	P(4)-O(17)	1.527(4) [1.275]
Ga(4)-O(10)#2	1.809(4) [0.807]	P(4)-O(16)	1.561(4) [1.163]
Ga(4)-O(17)#3	1.810(4) [0.805]	Σ(P(4)-O)	**5.154**
Ga(4)-O(17)	1.810(4)[0.805]		

O(4)-Ga(1)-O(5)	89.20(16)	O(10)#1-Ga(4)-O(10)#2	109.3(3)
O(4)-Ga(1)-O(6)	88.52(17)	O(10)#1-Ga(4)-O(17)#3	116.96(18)
O(5)-Ga(1)-O(6)	92.46(16)	O(10)#2-Ga(4)-O(17)#3	104.06(17)
O(4)-Ga(1)-O(3)	173.81(16)	O(10)#1-Ga(4)-O(17)	104.06(17)
O(5)-Ga(1)-O(3)	96.58(15)	O(10)#2-Ga(4)-O(17)	116.96(18)
O(6)-Ga(1)-O(3)	89.03(16)	O(17)#3-Ga(4)-O(17)	106.0(3)
O(4)-Ga(1)-O(2)	93.63(17)	O(5)-P(1)-O(7)	114.2(2)
O(5)-Ga(1)-O(2)	88.11(15)	O(5)-P(1)-O(3)#4	112.0(2)
O(6)-Ga(1)-O(2)	177.78(16)	O(7)-P(1)-O(3)#4	110.5(2)
O(3)-Ga(1)-O(2)	88.77(15)	O(5)-P(1)-O(15)#5	107.9(2)
O(4)-Ga(1)-O(1)	89.07(16)	O(7)-P(1)-O(15)#5	105.8(2)
O(5)-Ga(1)-O(1)	176.49(16)	O(3)#4-P(1)-O(15)#5	105.9(2)
O(6)-Ga(1)-O(1)	90.55(15)	O(2)#4-P(2)-O(11)	108.0(2)
O(3)-Ga(1)-O(1)	85.27(15)	O(2)#4-P(2)-O(9)	117.4(2)
O(2)-Ga(1)-O(1)	88.95(15)	O(11)-P(2)-O(9)	108.6(2)
O(6)-Ga(2)-O(9)	115.58(17)	O(2)#4-P(2)-O(10)	110.3(2)
O(6)-Ga(2)-O(12)	120.02(16)	O(11)-P(2)-O(10)	110.3(2)
O(9)-Ga(2)-O(12)	124.20(17)	O(9)-P(2)-O(10)	102.1(2)
O(6)-Ga(2)-O(7)	95.87(16)	O(1)#6-P(3)-O(12)	111.5(2)
O(9)-Ga(2)-O(7)	91.05(16)	O(1)#6-P(3)-O(13)	110.7(2)
O(12)-Ga(2)-O(7)	87.91(15)	O(12)-P(3)-O(13)	106.8(2)
O(6)-Ga(2)-O(8)	88.87(16)	O(1)#6-P(3)-O(14)#5	107.6(2)
O(9)-Ga(2)-O(8)	85.01(16)	O(12)-P(3)-O(14)#5	111.4(2)
O(12)-Ga(2)-O(8)	91.52(15)	O(13)-P(3)-O(14)#5	108.8(2)
O(7)-Ga(2)-O(8)	174.82(16)	O(4)#5-P(4)-O(8)#7	112.6(2)
O(13)-Ga(3)-O(15)	107.97(16)	O(4)#5-P(4)-O(17)	113.2(2)
O(13)-Ga(3)-O(16)	99.70(16)	O(8)#7-P(4)-O(17)	106.5(2)
O(15)-Ga(3)-O(16)	113.28(17)	O(4)#5-P(4)-O(16)	108.5(2)
O(13)-Ga(3)-O(14)	109.00(17)	O(8)#7-P(4)-O(16)	108.3(2)
O(15)-Ga(3)-O(14)	116.28(16)	O(17)-P(4)-O(16)	107.5(2)
O(16)-Ga(3)-O(14)	109.24(16)		

Values in brackets are the bond valences. Their sum BVS appears in bold type at the end of the list of the distances around every cations. Symmetry transformations used to generate equivalent atoms. **1**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+1,-z; #3 -x,-y+2,-z. **2**: #1 -x+1,-y,-z; #2 -x+1,-y,-z+1; #3 x,y-1,z; #4 -x+2,-y,-z; #5 -x+1,-y-1,-z. **3**: #1 -x+1,-y,-z+1; #2 x+1,y,z; #3 -x+1,-y+1,-z+1; #4 -x+1,-y+1,-z+2; #5 -x+1,-y,-z+2. **4**: #1 x+1,-y+3/2,z+1/2; #2 x+1,y,z+1; #3 x,-y+3/2,z+1/2; #4 x,-y+3/2,z-1/2. **5**: #1 -x,y+1,-z+1/2; #2 x,y+1,z; #3 -x,y,-z+1/2; #4 -x,-y-1,-z+1; #5 -x,-y,-z+1; #6 -x-1/2,-y-1/2,-z+1; #7 x+1/2,y+1/2,z.