Table 1. Crystal data and structure refinement for (ma)$Zn_4(PO_4)_3$.

Identification code		Zn4P3
Empirical formula		$CH_6NO_{12}P_3Zn_4$
Formula weight		578.46
Temperature		295(2) K
Crystal size		$0.29 \times 0.14 \times 0.09$ mm^3
Crystal habit		colorless prism
Crystal system		Orthorhombic
Space group		*Pbca*
Unit cell dimensions		a = 14.6797(6) Å α = 90°
		b = 10.1204(4) Å β = 90°
		c = 16.6015(7) Å γ = 90°
Volume		2466.39(17) Å^3
Z		8
Density, ρ_{calc}		3.116 g/cm^3
Absorption coefficient, μ		8.140 mm^{-1}
F(000)		2240 e
Diffractometer		Bruker Smart Apex CCD area detector
Radiation source		fine-focus sealed tube, MoKα, 0.71073 Å
θ range for data collection		2.45 to 30.51°
Index ranges		$-20 \le h \le 20$, $-14 \le k \le 14$, $-23 \le l \le 23$
Reflections collected		27937
Independent reflections		3750
Observed reflection, I>2σ(I)		3409
Coverage of independent reflections		99.6 %
Variation in check reflections		0.05 %
Absorption correction		Semi-empirical from equivalents SADABS
Max. and min. transmission		0.4807 and 0.2750
Structure solution technique		direct
Refinement technique		Full-matrix least-squares on F^2
Function minimized		$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters		3750 / 6 / 217
Goodness-of-fit on F^2		1.043
Δ/σ_{max}		0.001
Final R indices:	R_1, I>2σ(I)	0.0240
	wR_2, all data	0.0555
	R_{int}	0.0413
	R_{sig}	0.0251
Extinction coefficient		0.00128(8)
Largest diff. peak and hole		0.591 and -0.467 e/Å^3

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 2. Atomic coordinates and equivalent* isotropic atomic displacement parameters ($Å^2$) for $(ma)Zn_4(PO_4)_3$.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Zn1	0.143310(17)	0.87693(2)	0.226671(15)	0.01001(7)
Zn2	0.365668(17)	0.89255(2)	0.195273(16)	0.00995(7)
Zn3	0.448530(18)	1.15139(2)	0.089206(16)	0.01154(7)
Zn4	0.431142(18)	0.65219(3)	0.058045(16)	0.01128(7)
P1	0.25741(4)	0.62824(5)	0.16315(3)	0.00832(10)
P2	0.55109(4)	0.88202(5)	0.10500(3)	0.00902(11)
P3	0.53918(4)	0.39803(5)	0.12570(3)	0.00910(11)
O1	0.25332(10)	0.77675(16)	0.18759(10)	0.0119(3)
O2	0.05174(11)	0.82628(17)	0.14889(11)	0.0159(3)
O3	0.19700(12)	1.05113(16)	0.23111(10)	0.0159(3)
O4	0.11792(11)	0.82320(17)	0.33431(10)	0.0149(3)
O5	0.34181(10)	1.07592(15)	0.15445(10)	0.0114(3)
O6	0.45376(11)	0.82081(16)	0.11795(10)	0.0135(3)
O7	0.39314(13)	0.89155(19)	0.30601(10)	0.0209(4)
O8	0.54329(12)	1.02991(16)	0.11857(12)	0.0189(4)
O9	0.41612(12)	1.15847(19)	-0.02184(10)	0.0192(4)
O10	0.30641(12)	0.61394(17)	0.08388(11)	0.0173(3)
O11	0.52127(13)	0.53793(16)	0.10017(12)	0.0218(4)
O12	0.42425(11)	0.68738(17)	-0.05594(9)	0.0145(3)
C1	0.2458(2)	0.5902(4)	0.4616(2)	0.0314(7)
N1	0.26675(16)	0.6706(2)	0.39028(14)	0.0199(4)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters* ($Å^2$) for $(ma)Zn_4(PO_4)_3$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	0.00913(12)	0.01139(12)	0.00950(12)	0.00012(9)	0.00052(9)	-0.00084(9)
Zn2	0.00925(12)	0.01063(12)	0.00998(12)	0.00013(9)	-0.00003(9)	0.00008(9)
Zn3	0.01341(13)	0.01137(12)	0.00984(12)	-0.00063(9)	0.00031(9)	0.00149(9)
Zn4	0.01215(13)	0.01184(12)	0.00986(12)	-0.00049(9)	0.00123(9)	0.00008(9)
P1	0.0075(2)	0.0074(2)	0.0101(2)	-0.00065(18)	-0.00002(19)	-0.00014(17)
P2	0.0083(2)	0.0101(2)	0.0087(2)	-0.00063(18)	-0.00071(19)	0.00063(18)
P3	0.0092(2)	0.0093(2)	0.0088(2)	-0.00031(18)	-0.00020(19)	0.00007(19)
O1	0.0094(7)	0.0094(7)	0.0168(8)	-0.0010(6)	0.0000(6)	-0.0007(5)
O2	0.0133(8)	0.0154(8)	0.0189(8)	-0.0042(6)	-0.0072(6)	0.0036(6)
O3	0.0182(8)	0.0127(7)	0.0169(8)	0.0000(6)	0.0065(7)	-0.0039(6)
O4	0.0155(8)	0.0189(8)	0.0105(7)	0.0033(6)	0.0048(6)	0.0057(6)
O5	0.0093(7)	0.0103(7)	0.0147(8)	0.0023(6)	0.0003(6)	0.0019(6)
O6	0.0096(7)	0.0138(7)	0.0170(8)	-0.0050(6)	0.0034(6)	-0.0022(6)
O7	0.0209(9)	0.0296(10)	0.0122(8)	0.0019(7)	-0.0065(7)	-0.0021(7)
O8	0.0147(8)	0.0098(7)	0.0323(10)	-0.0016(7)	-0.0045(7)	0.0013(6)
O9	0.0165(8)	0.0333(10)	0.0078(7)	-0.0018(7)	0.0017(6)	0.0008(7)
O10	0.0134(8)	0.0232(9)	0.0151(8)	-0.0057(6)	0.0064(6)	-0.0056(7)
O11	0.0199(9)	0.0115(8)	0.0340(11)	0.0048(7)	-0.0046(8)	0.0019(7)
O12	0.0170(8)	0.0180(8)	0.0084(7)	-0.0015(6)	0.0019(6)	0.0036(6)
C1	0.0273(15)	0.0343(16)	0.0326(16)	0.0136(13)	0.0003(13)	0.0006(13)
N1	0.0174(11)	0.0214(11)	0.0209(11)	0.0028(9)	0.0000(9)	0.0023(9)

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table 4. Hydrogen atom coordinates and isotropic atomic displacement parameters ($Å^2$) for $(ma)Zn_4(PO_4)_3$.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H1C	0.297(3)	0.544(4)	0.477(3)	0.078(15)
H2C	0.220(4)	0.645(4)	0.500(3)	0.09(2)
H3C	0.205(3)	0.526(4)	0.442(3)	0.084(17)
H1N	0.3098(18)	0.719(3)	0.3998(19)	0.026(9)
H2N	0.2212(19)	0.713(3)	0.378(2)	0.038(10)
H3N	0.284(2)	0.627(3)	0.3522(18)	0.032(10)

Table 5. Bond lengths [Å] and angles [°] for (ma)$Zn_4(PO_4)_3$.

Zn(1)-O(4)	1.9047(16)	O(7)-Zn(2)-O(6)	119.74(8)
Zn(1)-O(3)	1.9325(16)	O(7)-Zn(2)-O(5)	111.85(7)
Zn(1)-O(2)	1.9331(16)	O(6)-Zn(2)-O(5)	103.67(7)
Zn(1)-O(1)	2.0141(15)	O(7)-Zn(2)-O(1)	103.46(7)
Zn(2)-O(7)	1.8821(17)	O(6)-Zn(2)-O(1)	106.33(6)
Zn(2)-O(6)	1.9614(16)	O(5)-Zn(2)-O(1)	111.80(6)
Zn(2)-O(5)	2.0065(15)	O(9)-Zn(3)-O(8)	116.79(8)
Zn(2)-O(1)	2.0272(15)	O(9)-Zn(3)-O(2)#1	116.06(8)
Zn(3)-O(9)	1.9053(17)	O(8)-Zn(3)-O(2)#1	115.86(7)
Zn(3)-O(8)	1.9195(17)	O(9)-Zn(3)-O(5)	109.52(7)
Zn(3)-O(2)#1	2.0284(17)	O(8)-Zn(3)-O(5)	100.42(7)
Zn(3)-O(5)	2.0520(16)	O(2)#1-Zn(3)-O(5)	93.75(6)
Zn(4)-O(11)	1.8912(17)	O(11)-Zn(4)-O(10)	117.47(8)
Zn(4)-O(10)	1.9201(17)	O(11)-Zn(4)-O(12)	120.84(8)
Zn(4)-O(12)	1.9283(16)	O(10)-Zn(4)-O(12)	101.91(7)
Zn(4)-O(6)	2.0029(16)	O(11)-Zn(4)-O(6)	102.79(7)
P(1)-O(10)	1.5066(17)	O(10)-Zn(4)-O(6)	102.65(7)
P(1)-O(3)#2	1.5265(17)	O(12)-Zn(4)-O(6)	109.79(7)
P(1)-O(5)#2	1.5565(16)	O(10)-P(1)-O(3)#2	112.78(10)
P(1)-O(1)	1.5580(16)	O(10)-P(1)-O(5)#2	109.46(9)
P(2)-O(8)	1.5179(17)	O(3)#2-P(1)-O(5)#2	107.76(9)
P(2)-O(9)#3	1.5183(18)	O(10)-P(1)-O(1)	109.79(9)
P(2)-O(4)#4	1.5270(17)	O(3)#2-P(1)-O(1)	108.52(9)
P(2)-O(6)	1.5721(16)	O(5)#2-P(1)-O(1)	108.43(8)
P(3)-O(11)	1.5011(17)	O(8)-P(2)-O(9)#3	115.15(11)
P(3)-O(7)#5	1.5089(18)	O(8)-P(2)-O(4)#4	109.56(10)
P(3)-O(12)#6	1.5417(17)	O(9)#3-P(2)-O(4)#4	106.93(10)
P(3)-O(2)#2	1.5675(17)	O(8)-P(2)-O(6)	107.44(9)
P(3)-Zn(3)#7	2.8928(6)	O(9)#3-P(2)-O(6)	107.83(10)
C(1)-N(1)	1.469(4)	O(4)#4-P(2)-O(6)	109.88(10)
		O(11)-P(3)-O(7)#5	111.62(11)
O(4)-Zn(1)-O(3)	107.72(7)	O(11)-P(3)-O(12)#6	112.19(10)
O(4)-Zn(1)-O(2)	114.51(8)	O(7)#5-P(3)-O(12)#6	108.10(10)
O(3)-Zn(1)-O(2)	123.43(7)	O(11)-P(3)-O(2)#2	110.92(10)
O(4)-Zn(1)-O(1)	108.39(7)	O(7)#5-P(3)-O(2)#2	110.86(10)
O(3)-Zn(1)-O(1)	98.31(7)	O(12)#6-P(3)-O(2)#2	102.78(9)
O(2)-Zn(1)-O(1)	102.06(7)	O(11)-P(3)-Zn(3)#7	132.39(8)

O(7)#5-P(3)-Zn(3)#7	115.01(8)	P(1)#1-O(5)-Zn(3)	129.55(9)
O(12)#6-P(3)-Zn(3)#7	61.25(7)	Zn(2)-O(5)-Zn(3)	112.91(7)
O(2)#2-P(3)-Zn(3)#7	42.27(6)	P(2)-O(6)-Zn(2)	122.88(9)
P(1)-O(1)-Zn(1)	126.90(9)	P(2)-O(6)-Zn(4)	114.74(9)
P(1)-O(1)-Zn(2)	122.87(9)	Zn(2)-O(6)-Zn(4)	122.08(8)
Zn(1)-O(1)-Zn(2)	109.94(7)	P(3)#9-O(7)-Zn(2)	151.02(13)
P(3)#1-O(2)-Zn(1)	129.29(10)	P(2)-O(8)-Zn(3)	130.43(11)
P(3)#1-O(2)-Zn(3)#2	106.42(9)	P(2)#3-O(9)-Zn(3)	142.23(12)
Zn(1)-O(2)-Zn(3)#2	123.99(8)	P(1)-O(10)-Zn(4)	129.13(11)
P(1)#1-O(3)-Zn(1)	128.10(10)	P(3)-O(11)-Zn(4)	143.48(12)
P(2)#8-O(4)-Zn(1)	129.31(10)	P(3)#6-O(12)-Zn(4)	127.98(10)
P(1)#1-O(5)-Zn(2)	116.53(9)		

Symmetry transformations: #1 -x+1/2,y+1/2,z #2 -x+1/2,y-1/2,z #3 -x+1,-y+2,-z #4 x+1/2,y,-z+1/2 #5 -x+1,y-1/2,-z+1/2 #6 -x+1,-y+1,-z #7 x,y-1,z #8 x-1/2,y,-z+1/2 #9 -x+1,y+1/2,-z+1/2

Table 6. Hydrogen bonds for (ma)$Zn_4(PO_4)_3$ [Å and °].

D—H···A	d(D—H)	d(H···A)	d(D···A)	∠(DHA)
N1—H1N···O12#1	0.82(2)	2.06(2)	2.865(3)	167(3)
N1—H1N···O7	0.82(2)	2.64(3)	3.225(3)	130(3)
N1—H2N···O4	0.82(2)	2.02(2)	2.832(3)	172(4)
N1—H3N···O3#2	0.81(2)	2.17(3)	2.954(3)	163(3)

Symmetry transformations: #1 x,-y+3/2,z+1/2 #2 -x+1/2,y-1/2,

Table 7. Crystal data and structure refinement for $(ma)_2Zn_5(PO_4)_4$.

Identification code	Zn5P4	
Empirical formula	$C_2H_{12}N_2O_{16}P_4Zn_5$	
Formula weight	770.87	
Temperature	296 K	
Crystal size	$0.14 \times 0.03 \times 0.02$ mm^3	
Crystal habit	colorless needle	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.2590(19) Å	α = 90°
	b = 13.407(4) Å	β = 90°
	c = 18.031(5) Å	γ = 90°
Volume	1754.8(8) Å^3	
Z	4	
Density, ρ_{calc}	2.918 g/cm^3	
Absorption coefficient, μ	7.187 mm^{-1}	
F(000)	1504 $\bar{e}$	
Diffractometer	Bruker Smart Apex CCD area detector	
Radiation source	fine-focus sealed tube, MoKα, 0.71073 Å	
θ range for data collection	1.89 to 22.72°	
Index ranges	$-7 \leq h \leq 7$, $-14 \leq k \leq 14$, $-19 \leq l \leq 19$	
Reflections collected	11139	
Independent reflections	2336	
Observed reflection, I>2σ(I)	2128	
Coverage of independent reflections	98.6 %	
Variation in check reflections	0.1 %	
Absorption correction	Semi-empirical from equivalents XPREP	
Max. and min. transmission	0.8661 and 0.6969	
Structure solution technique	direct	
Refinement technique	Full-matrix least-squares on F^2	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	2336 / 0 / 188	
Goodness-of-fit on F^2	1.095	
Δ/σ_{max}	0.000	
Final R indices:	R_1, I>2σ(I)	0.0774
	wR_2, all data	0.1805
	R_{int}	0.1392
	R_{sig}	0.1083
Absolute structure parameter	0.0(8)	
Extinction coefficient	0.089(3)	
Largest diff. peak and hole	1.158 and -1.174 $\bar{e}$/Å^3	

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 8. Atomic coordinates and equivalent* isotropic atomic displacement parameters ($Å^2$) for $(ma)_2Zn_5(PO_4)_4$.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Zn1	0.4865(3)	0.61494(16)	0.20659(13)	0.0161(6)
Zn2	0.4992(3)	0.37066(17)	0.22291(12)	0.0175(6)
Zn3	0.1428(3)	-0.00154(18)	0.08123(12)	0.0164(5)
Zn4	-0.0536(3)	0.35794(18)	0.19721(13)	0.0176(6)
Zn5	-0.0576(3)	0.61190(17)	0.18609(13)	0.0176(6)
P1	0.6823(6)	0.4804(4)	0.0934(3)	0.0143(12)
P2	0.2604(8)	0.1908(4)	0.1709(3)	0.0166(13)
P3	0.2404(7)	-0.2113(4)	0.1526(3)	0.0150(13)
P4	0.1895(6)	0.4961(4)	0.2930(3)	0.0167(12)
O1	0.406(2)	0.7209(11)	0.1423(8)	0.026(4)
O2	0.5313(17)	0.4855(11)	0.1569(7)	0.022(3)
O3	0.303(2)	0.5893(11)	0.2814(9)	0.027(4)
O4	0.3046(19)	0.4033(11)	0.2904(8)	0.022(3)
O5	0.427(2)	0.2642(11)	0.1609(8)	0.026(4)
O6	0.2882(17)	0.1122(10)	0.1135(7)	0.014(3)
O7	0.0819(19)	0.0233(11)	-0.0212(8)	0.029(4)
O8	0.2384(18)	-0.1371(10)	0.0911(8)	0.021(3)
O9	-0.0936(16)	0.0052(11)	0.1334(7)	0.020(3)
O10	0.071(2)	0.2405(11)	0.1645(8)	0.027(4)
O11	-0.2590(19)	0.3408(11)	0.2713(8)	0.021(3)
O12	-0.2015(18)	0.3872(10)	0.1099(7)	0.017(3)
O13	0.0434(17)	0.4888(10)	0.2306(7)	0.021(3)
O14	-0.2010(19)	0.5719(11)	0.0987(8)	0.022(3)
O15	-0.2737(19)	0.6479(10)	0.2495(8)	0.022(3)
O16	0.060(2)	0.7309(10)	0.1525(7)	0.018(3)
N1	0.721(3)	0.7805(16)	0.0614(13)	0.049(7)
C1	0.688(4)	0.8629(19)	0.0179(13)	0.039(7)
N2	0.713(3)	0.1844(13)	0.0715(10)	0.028(5)
C2	0.665(5)	0.159(4)	-0.0023(16)	0.104(16)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 9. Anisotropic atomic displacement parameters* ($Å^2$) for $(ma)_2Zn_5(PO_4)_4$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	0.0155(12)	0.0153(12)	0.0174(12)	-0.0020(10)	0.0002(10)	0.0010(10)
Zn2	0.0150(12)	0.0182(13)	0.0193(13)	0.0007(10)	-0.0003(10)	0.0007(11)
Zn3	0.0169(11)	0.0179(12)	0.0143(12)	0.0030(11)	0.0032(9)	0.0005(12)
Zn4	0.0120(11)	0.0193(12)	0.0215(13)	0.0021(10)	-0.0014(10)	0.0034(11)
Zn5	0.0189(12)	0.0140(12)	0.0199(14)	0.0011(10)	-0.0011(10)	-0.0025(11)
P1	0.012(2)	0.017(3)	0.015(3)	0.003(2)	-0.0018(19)	0.000(2)
P2	0.016(3)	0.014(3)	0.020(3)	0.004(2)	-0.005(2)	-0.003(2)
P3	0.006(3)	0.017(3)	0.022(3)	0.000(2)	0.000(2)	-0.001(2)
P4	0.016(2)	0.021(3)	0.013(3)	-0.001(3)	0.0015(19)	-0.003(3)
N1	0.039(13)	0.052(13)	0.054(15)	0.042(12)	0.007(12)	0.009(12)
C1	0.053(16)	0.046(16)	0.018(13)	0.009(12)	-0.012(12)	0.003(15)
N2	0.034(11)	0.028(10)	0.021(11)	0.011(9)	0.014(9)	0.030(10)
C2	0.10(3)	0.19(4)	0.021(18)	0.00(2)	0.028(18)	0.09(3)

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table 10. Hydrogen atom coordinates and isotropic atomic displacement parameters ($Å^2$) for $(ma)_2Zn_5(PO_4)_4$.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H1A	0.7383	0.7275	0.0326	0.073
H1B	0.6243	0.7698	0.0909	0.073
H1C	0.8206	0.7909	0.0889	0.073
H1D	0.7579	0.8578	-0.0271	0.058
H1E	0.7235	0.9220	0.0443	0.058
H1F	0.5589	0.8663	0.0061	0.058
H2A	0.8264	0.1633	0.0812	0.042
H2B	0.6339	0.1556	0.1027	0.042
H2C	0.7074	0.2503	0.0770	0.042
H2D	0.5770	0.2061	-0.0210	0.156
H2E	0.6128	0.0933	-0.0033	0.156
H2F	0.7737	0.1604	-0.0328	0.156

Table 11. Bond lengths [Å] and angles [°] for $(ma)_2Zn_5(PO_4)_4$.

Zn(1)-O(1)	1.924(15)	O(1)-Zn(1)-O(3)	110.1(6)
Zn(1)-O(3)	1.926(16)	O(1)-Zn(1)-O(15)#1	110.0(6)
Zn(1)-O(15)#1	1.956(14)	O(3)-Zn(1)-O(15)#1	112.2(6)
Zn(1)-O(2)	1.980(14)	O(1)-Zn(1)-O(2)	115.1(6)
Zn(2)-O(5)	1.887(15)	O(3)-Zn(1)-O(2)	105.9(6)
Zn(2)-O(4)	1.915(14)	O(15)#1-Zn(1)-O(2)	103.4(6)
Zn(2)-O(2)	1.959(14)	O(5)-Zn(2)-O(4)	110.1(6)
Zn(2)-O(11)#1	2.001(14)	O(5)-Zn(2)-O(2)	105.5(6)
Zn(3)-O(7)	1.928(14)	O(4)-Zn(2)-O(2)	107.1(6)
Zn(3)-O(6)	1.943(13)	O(5)-Zn(2)-O(11)#1	110.6(6)
Zn(3)-O(8)	1.953(14)	O(4)-Zn(2)-O(11)#1	114.6(6)
Zn(3)-O(9)	1.959(12)	O(2)-Zn(2)-O(11)#1	108.5(6)
Zn(4)-O(10)	1.908(15)	O(7)-Zn(3)-O(6)	106.0(6)
Zn(4)-O(12)	1.946(14)	O(7)-Zn(3)-O(8)	109.3(6)
Zn(4)-O(13)	1.984(14)	O(6)-Zn(3)-O(8)	120.6(6)
Zn(4)-O(11)	2.015(14)	O(7)-Zn(3)-O(9)	104.5(6)
Zn(5)-O(16)	1.907(14)	O(6)-Zn(3)-O(9)	107.2(6)
Zn(5)-O(14)	1.963(15)	O(8)-Zn(3)-O(9)	108.1(6)
Zn(5)-O(13)	1.976(14)	O(10)-Zn(4)-O(12)	100.2(6)
Zn(5)-O(15)	2.001(14)	O(10)-Zn(4)-O(13)	131.0(6)
P(1)-O(7)#2	1.493(15)	O(12)-Zn(4)-O(13)	105.2(6)
P(1)-O(14)#1	1.493(15)	O(10)-Zn(4)-O(11)	117.4(6)
P(1)-O(12)#1	1.537(15)	O(12)-Zn(4)-O(11)	98.7(5)
P(1)-O(2)	1.587(14)	O(13)-Zn(4)-O(11)	99.3(6)
P(2)-O(6)	1.491(14)	O(16)-Zn(5)-O(14)	102.2(6)
P(2)-O(10)	1.535(16)	O(16)-Zn(5)-O(13)	131.4(6)
P(2)-O(15)#3	1.548(15)	O(14)-Zn(5)-O(13)	107.1(6)
P(2)-O(5)	1.570(16)	O(16)-Zn(5)-O(15)	109.3(6)
P(3)-O(8)	1.490(15)	O(14)-Zn(5)-O(15)	96.3(6)
P(3)-O(1)#4	1.519(16)	O(13)-Zn(5)-O(15)	105.1(6)
P(3)-O(16)#4	1.523(15)	O(7)#2-P(1)-O(14)#1	111.2(9)
P(3)-O(11)#3	1.545(15)	O(7)#2-P(1)-O(12)#1	114.1(8)
P(4)-O(4)	1.500(15)	O(14)#1-P(1)-O(12)#1	110.1(7)
P(4)-O(9)#5	1.504(14)	O(7)#2-P(1)-O(2)	107.1(8)
P(4)-O(3)	1.511(16)	O(14)#1-P(1)-O(2)	108.1(8)
P(4)-O(13)	1.550(14)	O(12)#1-P(1)-O(2)	105.9(8)
N(1)-C(1)	1.38(3)	O(6)-P(2)-O(10)	112.1(8)
N(2)-C(2)	1.42(4)	O(6)-P(2)-O(15)#3	111.9(8)
		O(10)-P(2)-O(15)#3	106.6(8)

O(6)-P(2)-O(5)	105.0(8)	P(4)-O(4)-Zn(2)	128.3(9)
O(10)-P(2)-O(5)	114.2(8)	P(2)-O(5)-Zn(2)	128.3(9)
O(15)#3-P(2)-O(5)	107.0(8)	P(2)-O(6)-Zn(3)	133.5(8)
O(8)-P(3)-O(1)#4	108.5(9)	P(1)#7-O(7)-Zn(3)	135.8(9)
O(8)-P(3)-O(16)#4	109.3(8)	P(3)-O(8)-Zn(3)	133.8(9)
O(1)#4-P(3)-O(16)#4	112.0(8)	P(4)#3-O(9)-Zn(3)	145.6(8)
O(8)-P(3)-O(11)#3	111.1(8)	P(2)-O(10)-Zn(4)	139.4(10)
O(1)#4-P(3)-O(11)#3	108.0(8)	P(3)#5-O(11)-Zn(2)#8	123.7(8)
O(16)#4-P(3)-O(11)#3	107.9(8)	P(3)#5-O(11)-Zn(4)	125.1(8)
O(4)-P(4)-O(9)#5	110.6(8)	Zn(2)#8-O(11)-Zn(4)	109.7(7)
O(4)-P(4)-O(3)	112.2(8)	P(1)#8-O(12)-Zn(4)	128.6(8)
O(9)#5-P(4)-O(3)	107.9(9)	P(4)-O(13)-Zn(5)	119.7(8)
O(4)-P(4)-O(13)	107.9(8)	P(4)-O(13)-Zn(4)	121.3(8)
O(9)#5-P(4)-O(13)	109.3(7)	Zn(5)-O(13)-Zn(4)	119.0(6)
O(3)-P(4)-O(13)	109.0(8)	P(1)#8-O(14)-Zn(5)	125.2(9)
P(3)#6-O(1)-Zn(1)	127.6(9)	P(2)#5-O(15)-Zn(1)#8	120.4(8)
P(1)-O(2)-Zn(2)	119.1(8)	P(2)#5-O(15)-Zn(5)	124.8(8)
P(1)-O(2)-Zn(1)	118.5(8)	Zn(1)#8-O(15)-Zn(5)	114.6(7)
Zn(2)-O(2)-Zn(1)	113.3(6)	P(3)#6-O(16)-Zn(5)	144.1(9)
P(4)-O(3)-Zn(1)	128.4(10)		

Symmetry transformations: #1 x+1,y,z #2 x+1/2,-y+1/2,-z #3 -x,y-1/2,-z+1/2 #4 x,y-1,z
#5 -x,y+1/2,-z+1/2 #6 x,y+1,z #7 x-1/2,-y+1/2,-z #8 x-1,y,z

Table 12. Hydrogen bonds for $(ma)_2Zn_5(PO_4)_4$ [Å and °].

D—H···A	d(D—H)	d(H···A)	d(D···A)	∠(DHA)
N1—H1A···O14#1	0.89	2.44	2.93(2)	115.0
N1—H1A···O8#2	0.89	2.54	3.36(3)	153.5
N1—H1B···O1	0.89	1.95	2.83(3)	167.7
N1—H1C···O16#1	0.89	2.23	3.03(3)	149.8
N1—H1C···O4#3	0.89	2.80	3.14(3)	104.7
N2—H2A···O9#1	0.89	2.39	3.00(2)	125.8
N2—H2A···O10#1	0.89	2.54	3.18(3)	129.3
N2—H2B···O5	0.89	2.34	2.84(2)	115.1
N2—H2B···O3#4	0.89	2.32	2.95(2)	127.6
N2—H2C···O12#1	0.89	2.04	2.87(2)	155.8

Symmetry transformations: #1 x+1,y,z #2 x+1/2,-y+1/2,-z #3 -x+1,y+1/2,-z+1/2 #4 -x+1,y-1/2,-z+1/2