Supporting Information

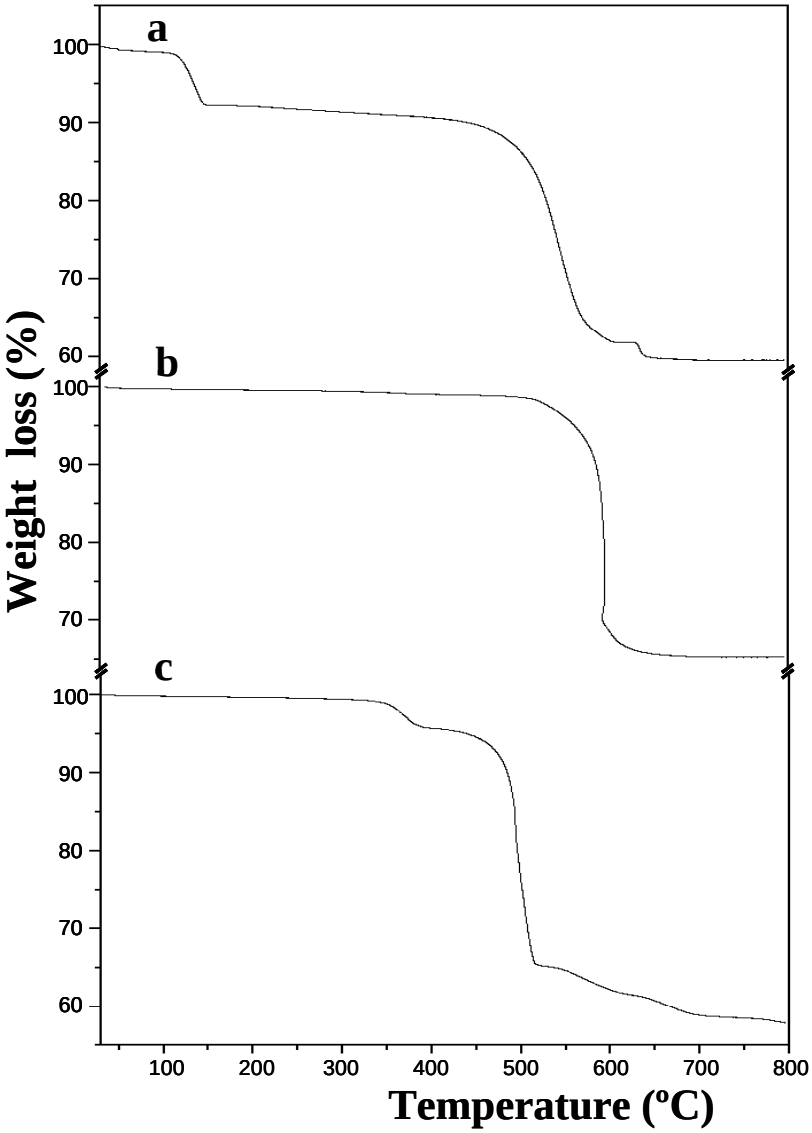

Figure S1. TGA curves for a) $Co_2(O_3PC_6H_4OC_6H_4PO_3)\cdot 2H_2O$, **VI**; b) $Zn_2(O_3PC_6H_4OC_6H_4PO_3)$, **X**; and c) $Zn(HO_3PC_6H_4OC_6H_4PO_3H)$, **XI**.

Supporting Information

Table S1. Atomic positional coordinates and equivalent isotropic displacement parameters for $[H_2O_3P\text{-}C_6H_4]_2\text{-}O$, **II**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	$U_{eq}/Å^2$
P1	0.4767(3)	0.1708(4)	0.5644(1)	0.026(1)
O1	0.5	-0.2443(11)	0.75	0.035(2)
O2	0.3380(7)	0.0528(9)	0.5378(2)	0.026(2)
O3	0.4480(6)	0.4298(8)	0.5684(2)	0.028(2)
O4	0.6542(6)	0.1309(7)	0.5429(2)	0.035(2)
C1	0.5001(11)	-0.1315(13)	0.7083(2)	0.024(2)
C2	0.5832(9)	-0.2370(14)	0.6727(3)	0.029(2)
C3	0.5739(10)	-0.1443(13)	0.6301(3)	0.026(2)
C4	0.4900(10)	0.0634(12)	0.6204(2)	0.020(2)
C5	0.4123(9)	0.1690(13)	0.6578(3)	0.025(2)
C6	0.4147(11)	0.0759(13)	0.7013(3)	0.024(2)
H1	0.3557	0.5035	0.5639	0.04
H2	0.6733	0.1069	0.5144	0.04
H3	0.6466	-0.3738	0.6778	0.04
H4	0.6271	-0.2239	0.6053	0.04
H5	0.3552	0.3112	0.6532	0.04
H6	0.3591	0.1514	0.7262	0.04

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Table S2. Refined atomic parameters for $Cu_2(O_3PC_4H_6OC_4H_6PO_3)$, **IX**, with a=8.1012(5) Å, b=5.3109(3) Å, c=29.260(1) Å and V=1258.9(2) $Å^3$ in S.G. Pbcn.

Atom	x	y	z	$U_{iso}/Å^2$
Cu	0.1829(3)	0.496(2)	0.0001(3)	0.056(2)
P	0.501(2)	0.585(1)	0.0582(1)	0.042(3)
O1	0.352(2)	0.421(4)	0.0438(4)	0.083(3)
O2	0.496(4)	0.841(1)	0.0331(2)	0.083(3)
O3	0.665(2)	0.448(5)	0.0491(4)	0.083(3)
C1	0.484(2)	0.646(2)	0.1191(1)	0.083(3)
C2	0.582(1)	0.524(2)	0.1515(2)	0.083(3)
C3	0.570(1)	0.591(2)	0.1980(2)	0.083(3)
C4	0.478(2)	0.801(2)	0.2115(1)	0.083(3)
C5	0.394(1)	0.937(2)	0.1772(2)	0.083(3)
C6	0.416(1)	0.879(2)	0.1313(2)	0.083(3)
O4	0.5000	0.932(2)	0.2500	0.083(3)

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Table S3. Positional parameters for $Zn(HO_3PC_4H_6OC_4H_6PO_3H)$, **XI**, with a=9.4991(9) Å, b=5.0445(5)Å, c=29.131(2) Å, γ=91.945(7)º and V=1395.1(3)$Å^3$, in S.G. $P112_1$.

Atom	x	y	z	Atom	x	y	z
Zn1	0.210(1)	0.131(3)	-0.027(0)	Zn1B	-0.164(1)	-0.159(3)	0.0335(5)
P1	0.424(2)	0.607(4)	-0.0751(8)	P1B	-0.386(2)	-0.627(4)	0.0645(8)
P2	-0.134(2)	0.042(4)	-0.0628(8)	P2B	0.158(2)	-0.131(4)	0.0595(7)
O1	0.573(3)	0.711(7)	-0.061(1)	O1B	-0.543(3)	-0.710(8)	0.062(2)
O2	0.384(4)	0.349(6)	-0.049(1)	O2B	-0.343(4)	-0.435(7)	0.025(1)
O3	0.313(4)	0.820(7)	-0.065(1)	O3B	-0.292(4)	-0.874(7)	0.062(1)
O4	-0.229(4)	0.283(6)	-0.067(1)	O4B	0.281(3)	-0.289(7)	0.040(1)
O5	-0.205(4)	-0.188(6)	-0.036(1)	O5B	0.149(4)	0.144(5)	0.0362(9)
O6	0.009(3)	0.126(7)	-0.041(1)	O6B	0.018(2)	-0.291(6)	0.055(1)
C1	0.423(5)	0.540(8)	-0.1358(9)	C1B	-0.355(5)	-0.461(8)	0.119(1)
C2	0.287(4)	0.465(12)	-0.151(2)	C2B	-0.339(7)	-0.611(11)	0.159(2)
C3	0.280(6)	0.387(13)	-0.198(2)	C3B	-0.409(8)	-0.538(13)	0.199(1)
C4	0.393(7)	0.250(13)	-0.216(2)	C4B	-0.458(7)	-0.281(14)	0.202(1)
C5	0.516(6)	0.226(10)	-0.189(2)	C5B	-0.477(7)	-0.132(10)	0.162(2)
C6	0.541(4)	0.423(12)	-0.156(1)	C6B	-0.444(7)	-0.246(10)	0.120(2)
C7	-0.097(4)	-0.072(8)	-0.1211(9)	C7B	0.193(5)	-0.072(8)	0.1202(8)
C8	-0.008(6)	0.077(10)	-0.152(1)	C8B	0.267(6)	-0.168(10)	0.159(1)
C9	-0.040(6)	0.068(10)	-0.199(1)	C9B	0.207(7)	-0.106(9)	0.2014(9)
C10	-0.081(8)	-0.184(13)	-0.216(1)	C10B	0.153(8)	0.149(9)	0.207(1)
C11	-0.159(8)	-0.355(11)	-0.187(2)	C11B	0.128(8)	0.299(8)	0.168(1)
C12	-0.176(7)	-0.282(10)	-0.141(1)	C12B	0.126(7)	0.170(10)	0.125(1)
O7	0.558(5)	0.844(8)	0.244(1)	O7B	0.107(6)	0.294(6)	0.243(1)

Table S4. Selected bond angles (º) for $Zn(HO_3PC_4H_6OC_4H_6PO_3H)$, **XI**.

O2-Zn1-O3	81.7(1)	O5-Zn1B-O2B	72.8(1)
O2-Zn1-O6	135.4(2)	O5-Zn1B-O3B	109.5(2)
O2-Zn1-O5B	121.2(2)	O5-Zn1B-O6B	116.9(2)
O3-Zn1-O6	110.5(2)	O2B-Zn1B-O3B	91.5(1)
O3-Zn1-O5B	130.8(2)	O2B-Zn1B-O6B	119.5(1)
O6-Zn1-O5B	84.0(1)	O3B-Zn1B-O6B	129.6(2)
O1-P1-O2	110.8(8)	O4-P2-O5	112.0(8)
O1-P1-O3	110.5(8)	O4-P2-O6	110.1(8)
O1-P1-C1	108.5(8)	O4-P2-C7	107.7(8)
O2-P1-O3	110.0(8)	O5-P2-O6	110.7(8)
O2-P1-C1	108.8(8)	O5-P2-C7	108.8(7)
O3-P1-C1	108.0(8)	O6-P2-C7	107.4(8)
O1B-P1B-O2B	111.7(8)	O4B-P2B-O5B	111.5(8)
O1B-P1B-O3B	110.9(8)	O4B-P2B-O6B	110.6(8)
O1B-P1B-C1B	108.2(8)	O4B-P2B-C7B	107.8(8)
O2B-P1B-O3B	109.2(8)	O5B-P2B-O6B	110.9(8)
O2B-P1B-C1B	108.8(8)	O5B-P2B-C7B	107.3(8)
O3B-P1B-C1B	108.0(8)	O6B-P2B-C7B	108.6(8)
C4-O7-C4B	130(6)		
C10-O7B-C10B	122(4)		