Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information for:

Systematic exploration of a rutile-type zinc(II)-phosphonocarboxylate open framework: the factors that influence the structure

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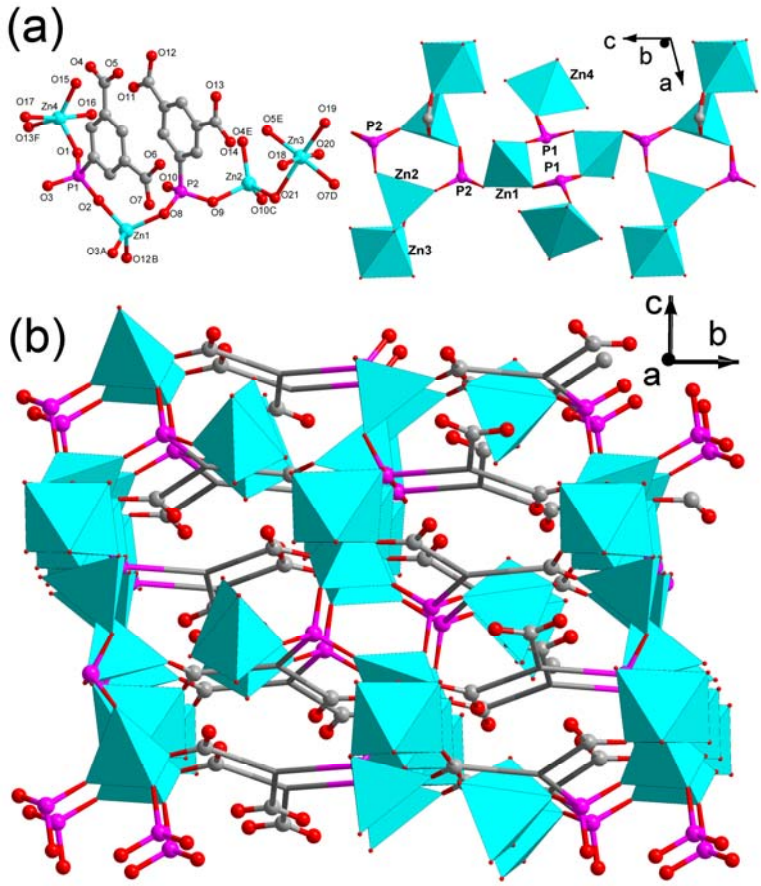
Table S1. Crystallographic data for **1-8**

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Formula	$C_{16}H_{24}O_{24}P_2Zn_5$	$C_{22}H_{21}P_2O_{19}NZn_3$	$C_{16}H_{12}O_{16}P_2Zn_3$	$C_{18}H_{19}O_{16}P_2NZn_3$	$C_{14}H_{27}N_4O_{10}PZn_2$	$C_{22}H_{32}N_4O16P_2Zn_3$	$C_{40}H_{54}O_{37}N_4P_4Zn_5$	$C_{20}H_{27}NO_{19}P_2Zn_3$
F.W.	989.14	861.45	718.31	763.39	573.11	866.57	1633.66	843.51
Space group	*P*-1	*Pbca*	*I*-42*d*	*C*2/*c*	$P2_1/c$	*C*2/*c*	*C*2/*c*	*I*-42*d*
a (Å)	7.419(3)	13.707(5)	18.310(6)	26.918(12)	9.866(3)	32.84(2)	28.54(2)	18.450(4)
b (Å)	9.969(3)	17.121(7)	18.310(6)	9.920(5)	15.449(5)	9.599(7)	12.983(7)	18.450(4)
c (Å)	11.148(4)	36.018(14)	23.222(11)	10.161(5)	17.097(4)	20.209(13)	15.834(9)	23.201(7)
α (^{o})	65.152(4)	90	90	90	90	90	90	90
β (^{o})	76.109(4)	90	90	112.179(6)	125.244(12)	106.710(9)	106.104(13)	90
γ (^{o})	69.965(4)	90	90	90	90	90	90	90
V(Å^3)	698.4(4)	8453(6)	7785(5)	2513(2)	2128.3(11)	6102(7)	5637(6)	7898(3)
Z	1	8	8	4	4	8	4	8
Dc (g cm^{-3})	2.352	1.354	1.226	1.983	1.789	1.887	1.904	1.400
μ(mm^{-1})	4.453	1.827	1.964	3.048	2.389	2.527	2.321	1.953
F(000)	492	3456	2848	1528	1176	3520	3296	3384
T(K)	293	293	293	293	293	293	293	293
Total collected	2946	33683	18703	4588	8819	12544	11544	16453
Unique data, R(int)	2458	7578, 0.117	3484, 0.0527	2224, 0.059	3815, 0.089	5496, 0.075	5047, 0.063	3567, 0.159
Observed [I > 2σ(I)]	1866	3977	3079	1734	3021	3801	3138	2916
GOF on F^2	0.93	0.94	1.18	1.01	0.94	0.87	0.87	0.99
R_1,[a] wR_2[b] [I>2σ(I)]	0.0337, 0.0809	0.0596, 0.1990	0.0399, 0.1462	0.0403, 0.1028	0.0456, 0.1046	0.0370, 0.0739	0.0393, 0.0896	0.0558, 0.1426
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	-0.73, 0.61	-0.59, 1.09	0.704, -0.493	-0.75, 1.09	-0.70, 0.89	-0.49, 0.58	-0.50, 1.09	-1.09, 0.76
CCDC	776920	751707	746203	776921	776922	776923	776924	776925

[a] $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. [b] $wR_2 = [\Sigma w(Fo^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

Figure S1. (a) the coordiantion geometry of Zn(II) ions in **1** (left) and the one dimensional inorganic chain (right) connected by phosphonate group; (b) the one dimensional chains further connected by tritopic pbdc ligands to generate the three dimensional structure of **1** (the phenyl group of pbdc has been reduced as 3-connected node, hydrogen atoms and lattice waters are omitted for clarity).



Fgure S2. (a) the one dimensional inorganic chain of **4** generated by corner-shared connected tetrahedral Zn(II) ions and phosphonate groups; (b) the coordination model of pbdc in **4**; (c) the three dimensional structure of **4** (the phenyl group of pbdc has been reduced as 3-connected node, hydrogen atoms, protonated teta and water molecules plus lattice waters are omitted for clarity).

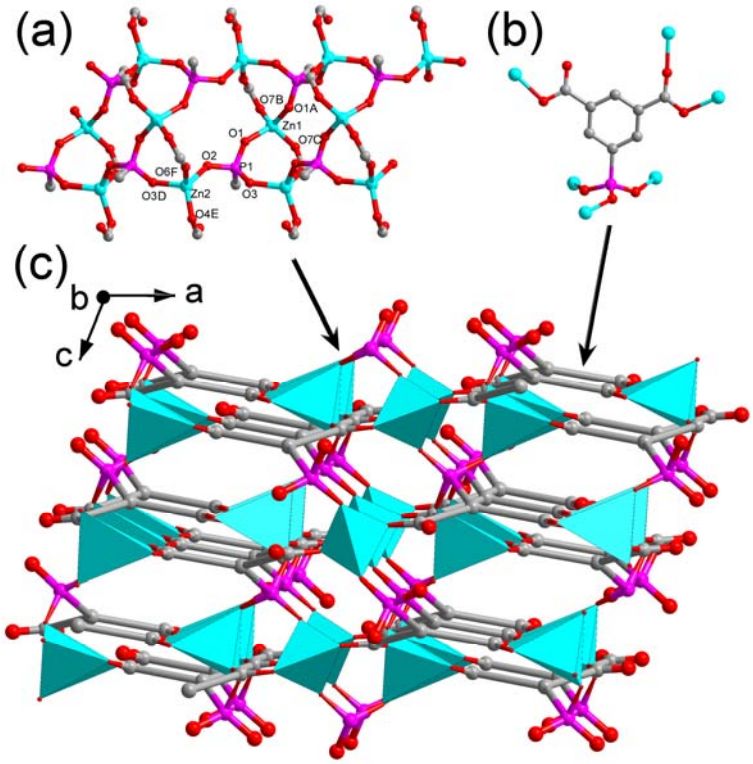


Figure S3. (a) the one-dimensional zigzag chain structure in **6**; (b) the coordination models of pbdc in **6**; (C) the three dimensional structure of **6** (the phenyl group of pbdc are reduced to the 3-connected node, hydrogen atoms and lattice waters are omitted for clarity)

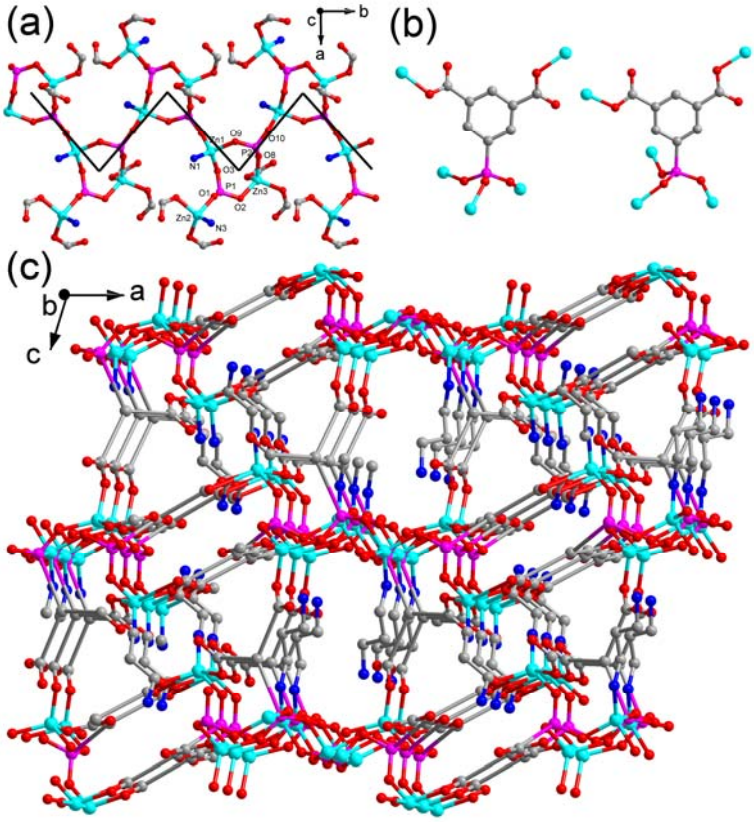


Figure S4. (a) the inorganic chain structure in structure **7**; (b) the coordination models of pbdc and Hpbdc ligands in structure **7**; (c) the three dimensional structure of **7** (the phenyl group of pbdc are reduced to the 3-connected node, hydrogen atoms and protonated *pz* plus lattice waters are omitted for clarity).

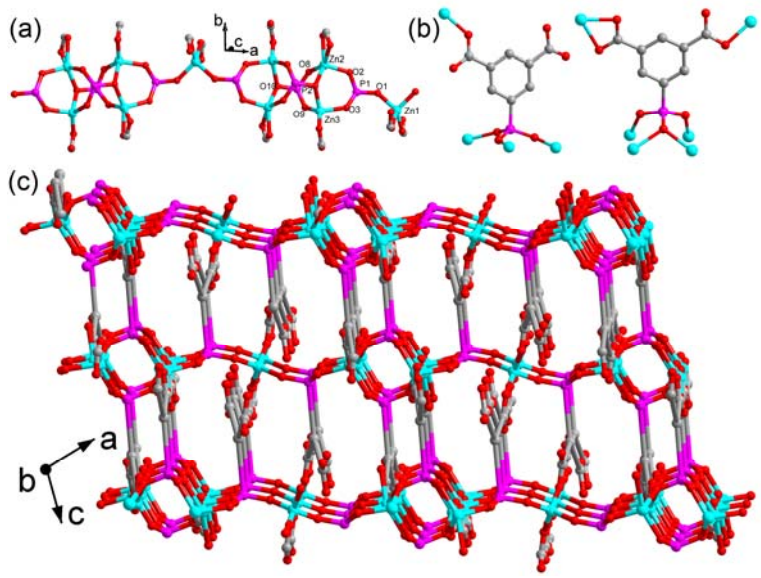


Figure S5. The TG curve of **8** (blue one)compared with that of **3** (black one).

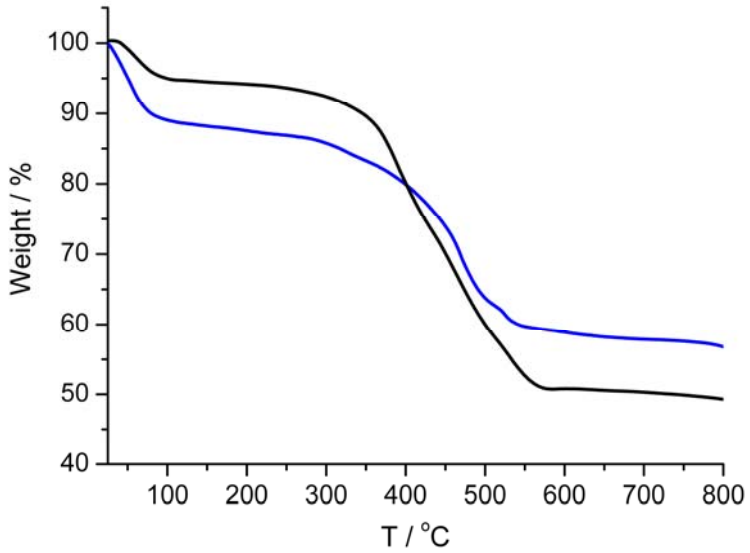


Figure S6. the PXRD data of **1** comapared with simulated one.

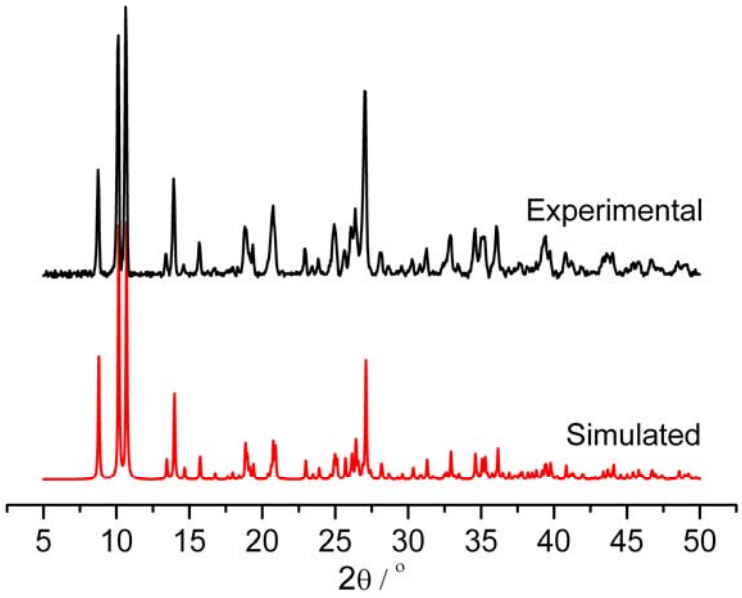
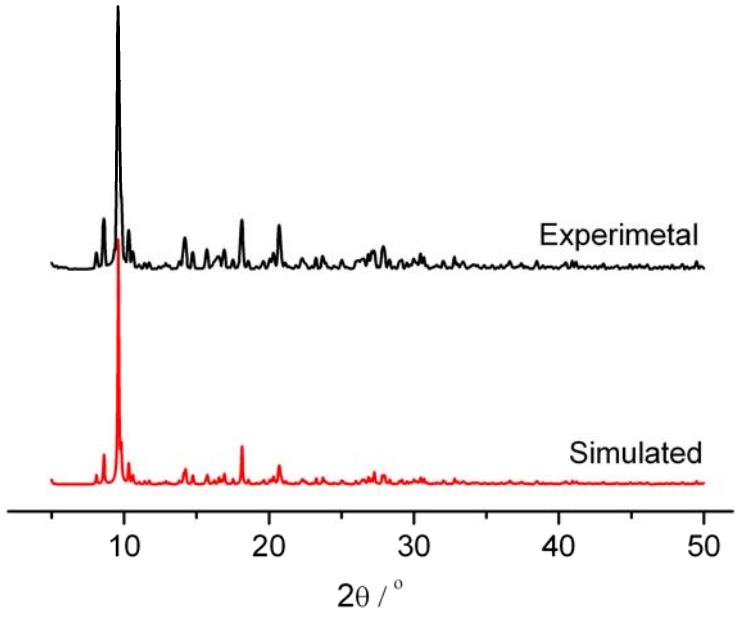


Figure S7. The PXRD data of **2** comapared with simulated one.



Figures S8. the PXRD data of **8** comapared with simulated one.