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Supplementary Material

Syntheses and characterizations of three organically templated zinc phosphites with 12-ring channels

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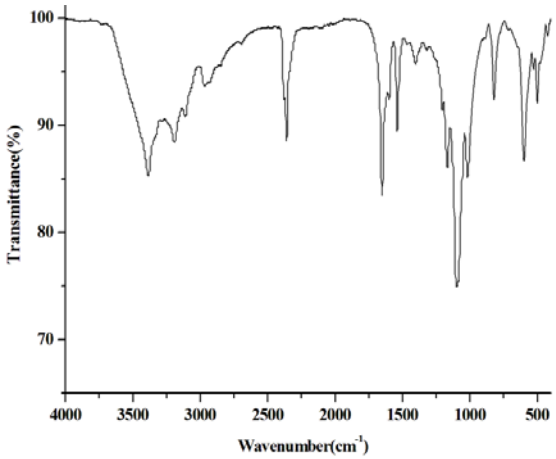

Fig. S1. IR spectrum of **1**.

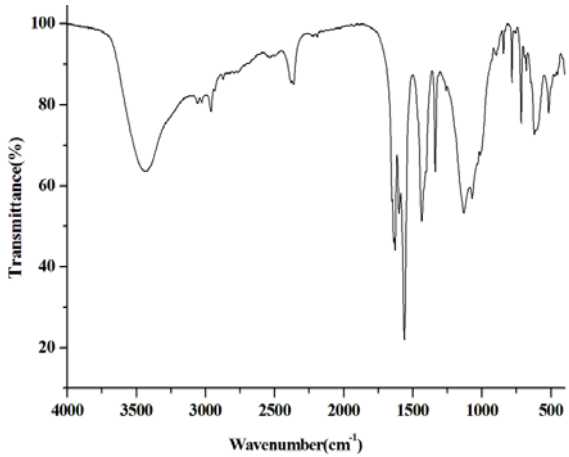

Fig. S2. IR spectrum of **2**.

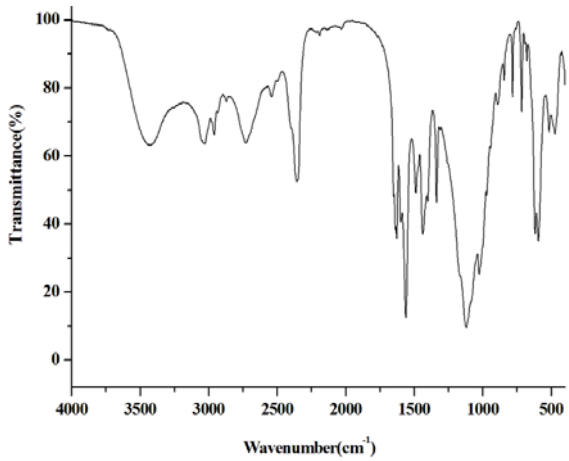

Fig. S3. IR spectrum of **3**.

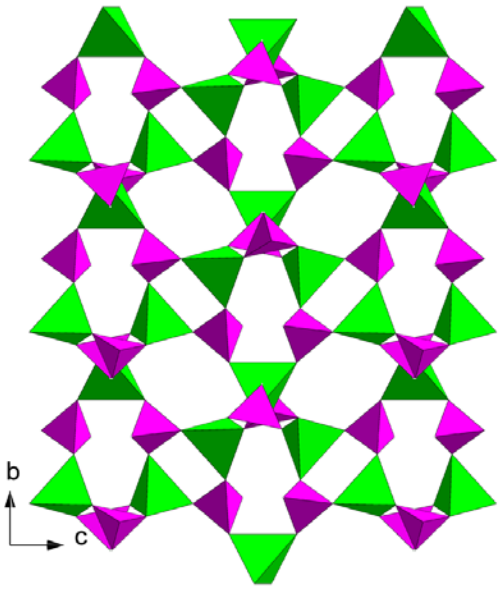

Fig. S4. Polyhedral view of the structure in **1** along the [100] direction with 8-ring windows. Color code: ZnO_4 tetrahedra, green; HPO_3 pseudopyramids, purple.

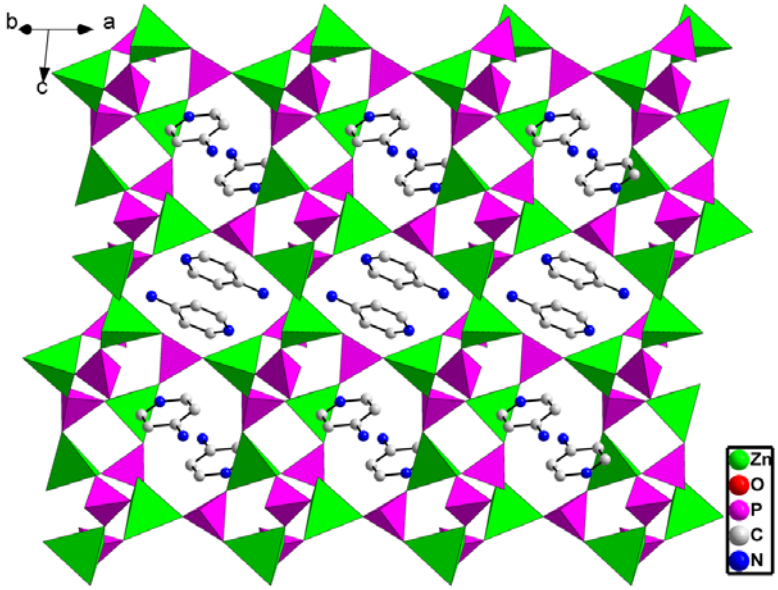

Fig. S5. Polyhedral view of the structure in **1** along the [110] direction with 8-ring windows, in which the SDAs reside.

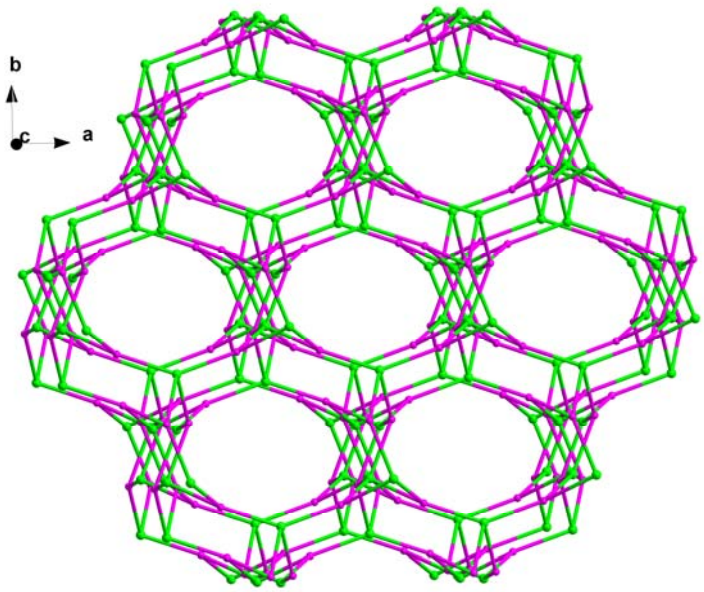

Fig. S6. The topology of **1**.

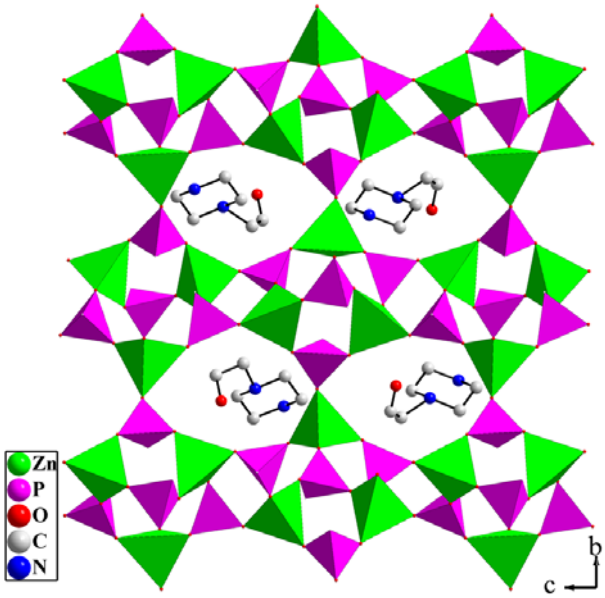

Fig. S7. Polyhedral view of the structure in **2** along the [100] direction with 8-ring windows, in which the SDAs reside. Color code: ZnO_4 tetrahedra, green; HPO_3 pseudopyramids, purple.

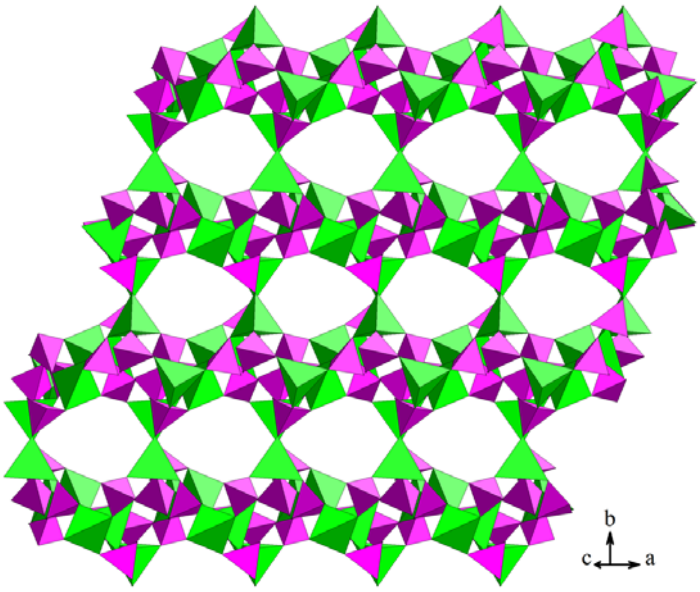

Fig. S8. Polyhedral view of the structure in **2** along the [101] direction with 8-ring windows. Color code: ZnO_4 tetrahedra, green; HPO_3 pseudopyramids, purple.

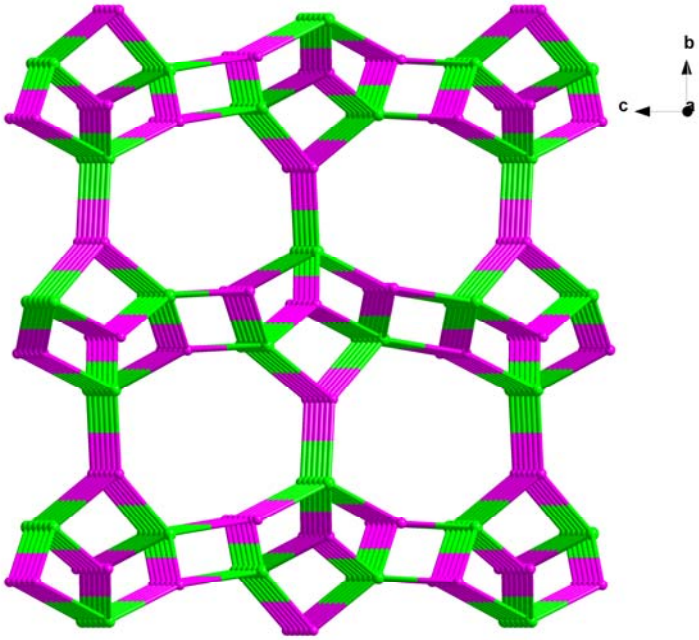

Fig. S9. The topology of **2**.

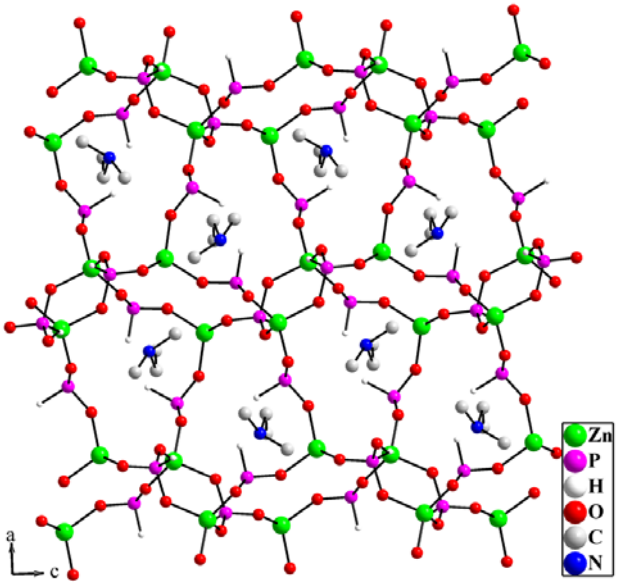

Fig. S10. View of the structure in **3** along the [101] direction with 8-ring windows, in which the SDAs reside.

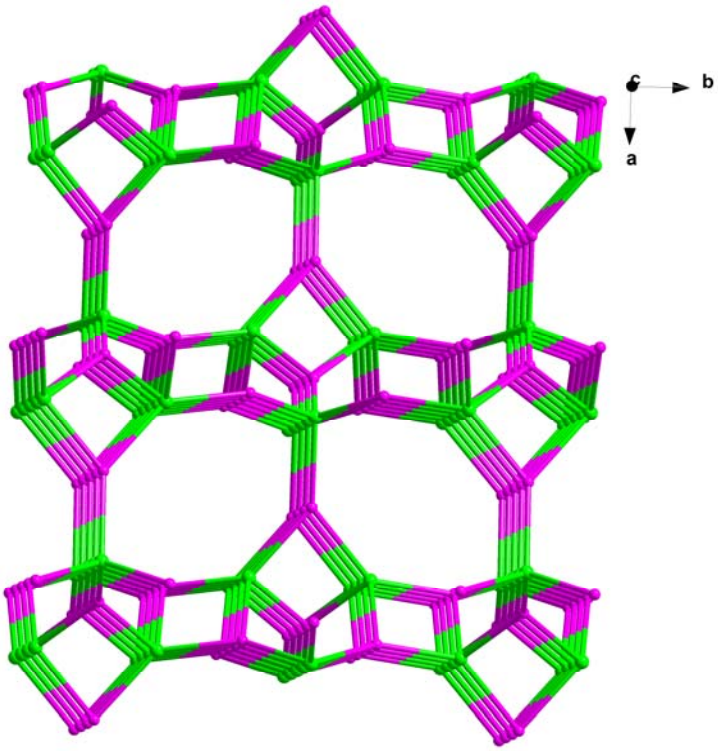

Fig. S11. The topology of **3**.

Table S1 Details of Hydrogen Bond Interactions in **1**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
N2-H2C...O1	0.86	2.07	2.917(4)	167.7
N2-H2B...O1	0.86	2.61	3.328(4)	141.8
N2-H2B...O6	0.86	2.26	3.070(4)	156.1
N1-H1B...O2	0.86	2.65	3.183(5)	121.3
N1-H1B...O4	0.86	2.06	2.869(4)	157.1

Table S2 Details of Hydrogen Bond Interactions in **2**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
O13-H13...O12	0.82	2.09	2.886(11)	163.8
O13'-H13'...O1	0.82	2.50	3.31(2)	169.0
N1-H1C...O2	0.90	1.87	2.763(6)	173.2
N1-H1D...O6	0.90	1.97	2.836(6)	159.7
N2-H2C...O12	0.95	2.28	3.064(7)	139.3
N2-H2C...O1	0.95	2.28	3.151(7)	152.7

Table S3 Details of Hydrogen Bond Interactions in **3**

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (deg)
N1-H1A...O1	0.95	1.83	2.757(7)	166.6