# Four new zinc (II) diphosphonates obtained via an ionothermal route: crystal structures and phase transformation behaviour

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## Supplementary Information

**Table S1** The elemental analysis results four compounds

| Compound | I | | | | | II | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Element | C | H | Zn | P | | C | H | Zn | P | |
| Theoretical Value (wt.%) | 24.46 | 2.05 | 33.29 | 15.78 | | 22.41 | 2.82 | 30.49 | 14.46 | |
| Observed value (wt.%) | 24.15 | 1.79 | 33.80 | 16.49 | | 22.79 | 2.91 | 31.08 | 15.01 | |
| Compound | III | | | | | IV | | | | |
| Element | C | H | Zn | P | Na | C | H | Zn | P | Na |
| Theoretical Value (wt.%) | 23.95 | 2.51 | 24.45 | 15.46 | 5.73 | 25.39 | 3.17 | 17.27 | 16.38 | 6.08 |
| Observed value (wt.%) | 24.21 | 2.59 | 25.08 | 16.15 | 6.10 | 25.40 | 3.30 | 17.96 | 16.99 | 6.67 |

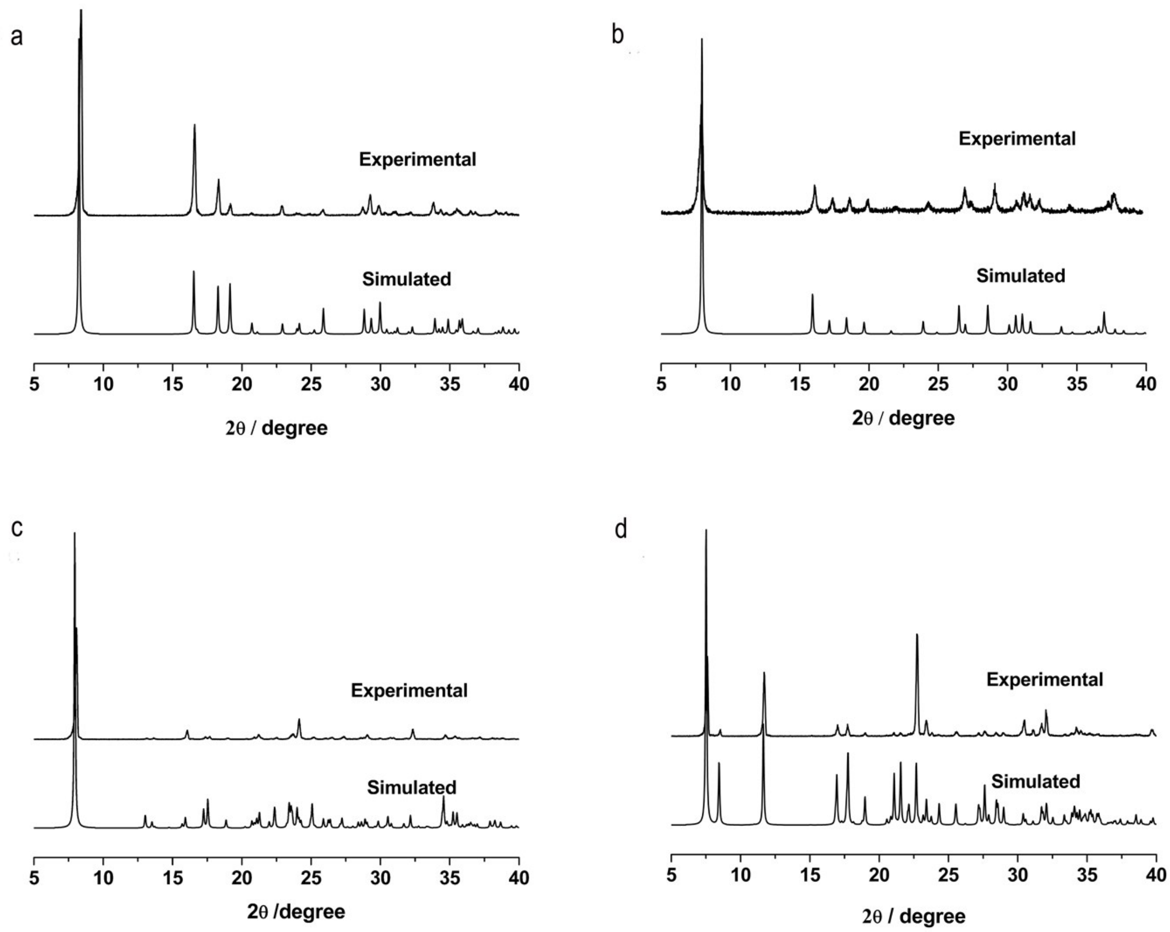


**Figure S1.** Simulated and experimental powder XRD patterns of compound I (a), II (b), III (c) and IV (d).

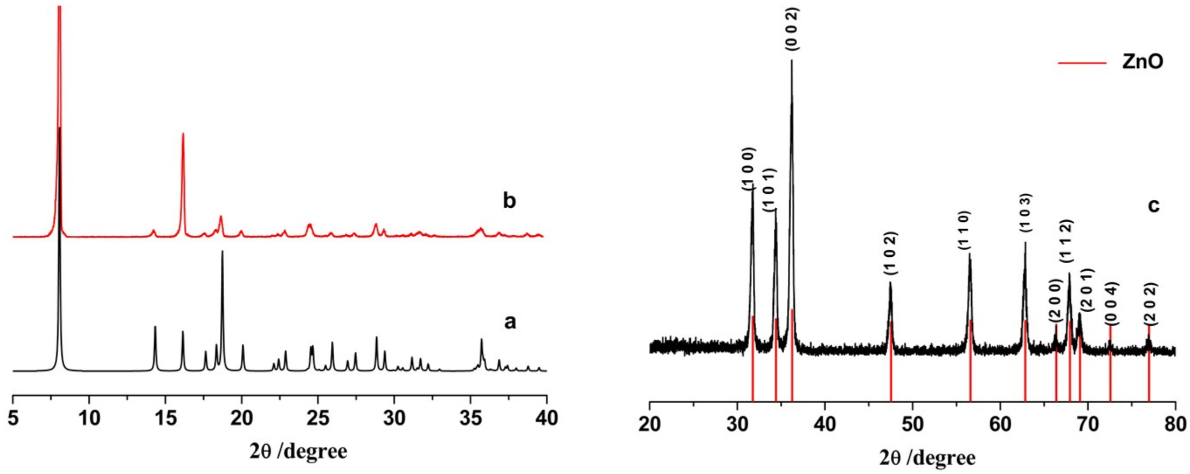


**Figure S2.** Powder XRD patterns of compound $Zn[HO_3PCH_2(C_6H_4)CH_2PO_3H]$ (a), experimental result with water as solvent(b), and experimental ZnO(c).

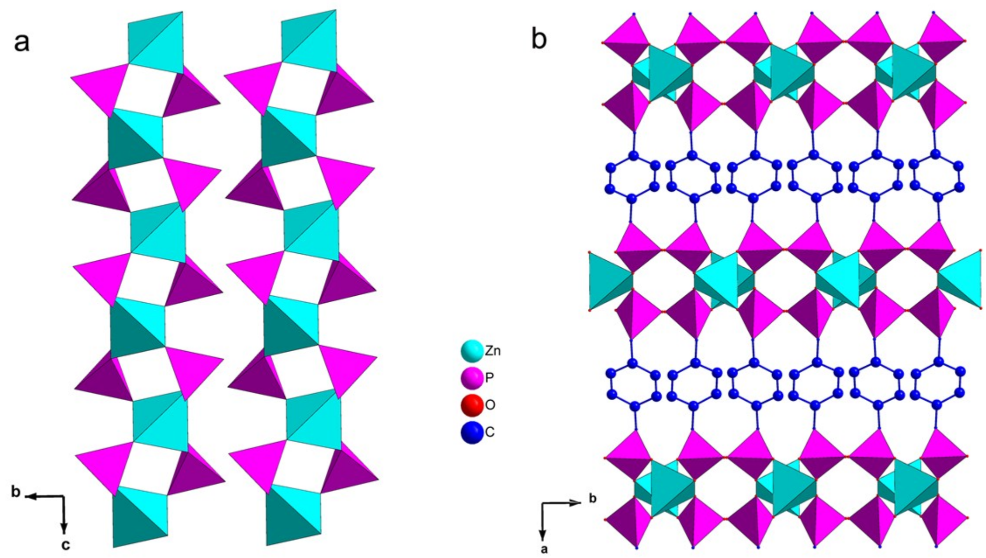


**Figure S3.** (a) Polyhedron representations of the 1D linear inorganic chain of compound $Zn[HO_3PCH_2(C_6H_4)CH_2PO_3H]$ running along *a*-axis. (b) Three-dimensional structure of compound $Zn[HO_3PCH_2(C_6H_4)CH_2PO_3H]$ in [001] direction[1].

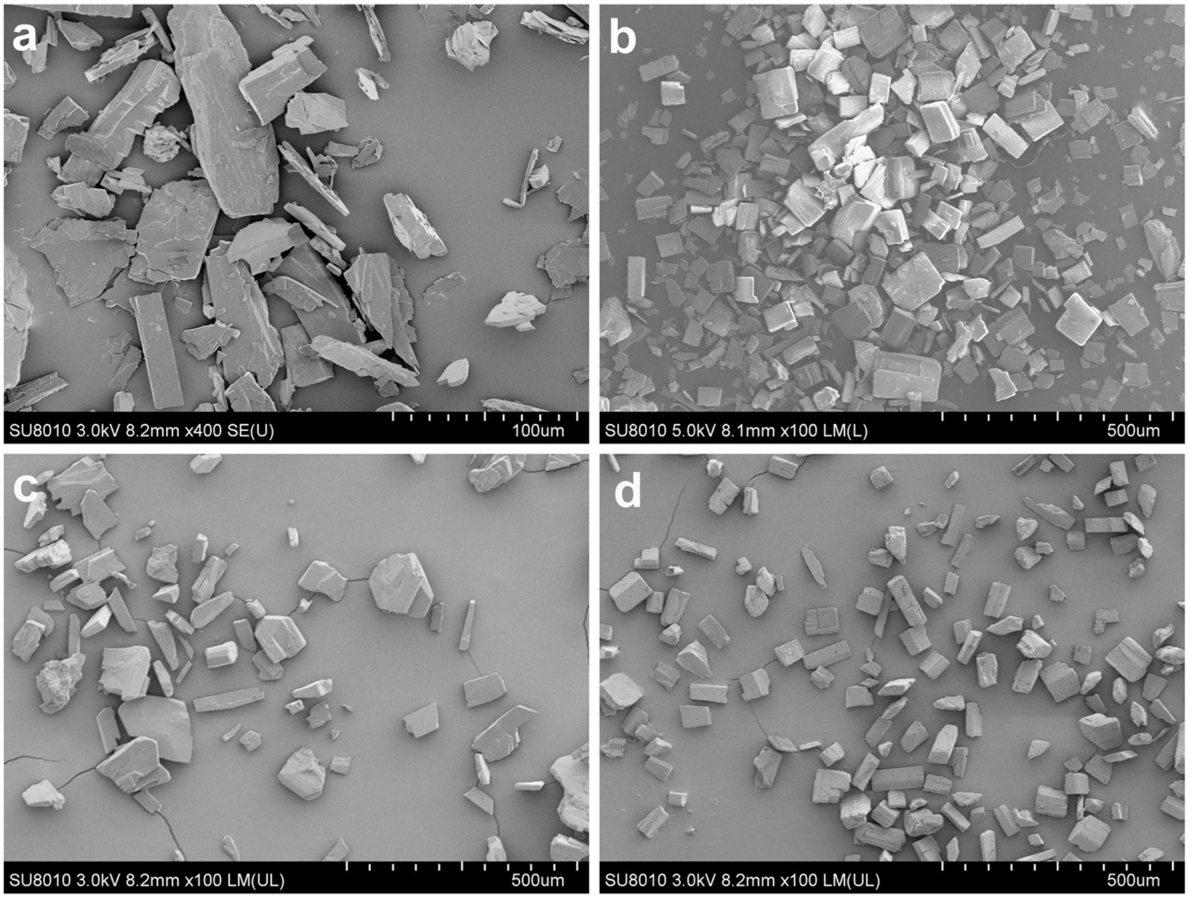


**Figure S4**. SEM images of compound I (a), II (b), III (c) and IV (d).

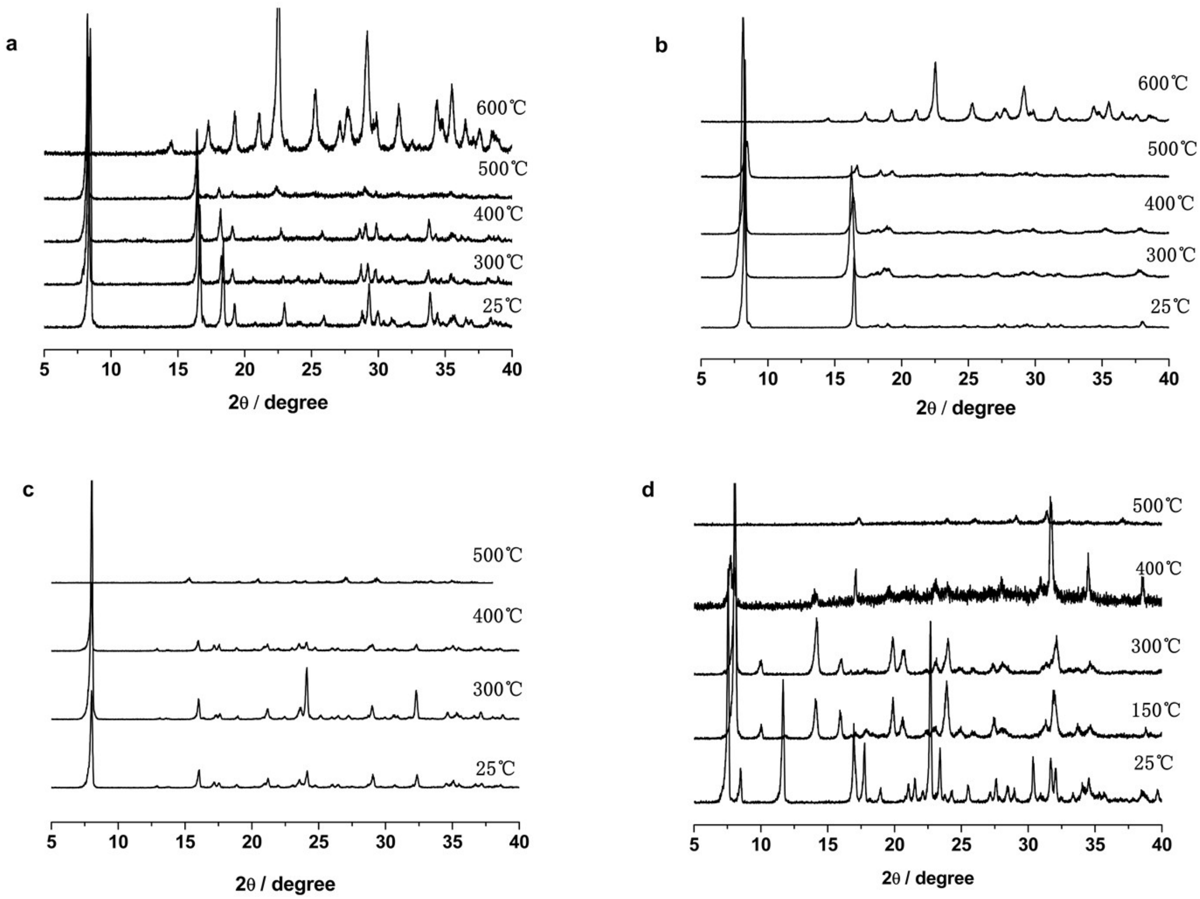


**Figure S5**. Powder XRD patterns of compound I (a), II (b), III (c) and IV (d) after calcination at different temperature.

## References

1 X. Z. Xu, P. Wang, R. Hao, M. N. Gan, F. X. Sun and G. S. Zhu, *Solid State Sci.,* 2009, **11**, 68.