*Supporting Information*

# A pillared-layered zincoborate with an anionic network containing unprecedented zinc oxide chains

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## Experimental Section

**Materials and physical measurements.** All chemicals and solvents in this study were commercially purchased and used without further purification. Elemental analyses of C, H and N were carried out with a Vario EL IIICHNOS elemental analyzer. IR spectra (KBr pellets) were recorded on an ABB Bomen $MB_{102}$ spectrometer over a range 400-4000 $cm^{-1}$. Thermal analyses were performed in air atmosphere with a heating rate of 10 ºC/min from 30 to 1000 ºC using a Mettler Toledo TGA/SDTA $851^e$ thermal analyzer. X-ray diffraction data were collected on an Agilent SuperNova Dual diffractometer with graphite-monochromated CuKα (λ = 1.54178 Å) radiation at room temperature. The program SADABS was used for the absorption correction. The structures were solved by the direct method and refined on $F^2$ by full-matrix least-squares methods using the SHELX97 program package. Powder XRD patterns were obtained using a Philips X'Pert-MPD diffractometer with $CuK_\alpha$ radiation (λ = 1.54056 Å). Diffuse-reflectance UV/Vis spectrum was recorded at room temperature on a PE Lambda 950 UV/Vis spectrophotometer in the wavelength range of 200-800 nm. $BaSO_4$ powder was used as 100% reflectance reference. The reflectance data were converted to absorbance using the Kubelka-Munk function: $\alpha/S = (1-R)^2/2R$, where $\alpha$ is the absorption coefficient, $S$ is the scattering coefficient, and $R$ is the reflectance.

## X-Ray data collection and structure refinement

Non-hydrogen atoms were refined anisotropically, and all hydrogen atoms bonded to C were generated geometrically. Crystallographic data and structural refinements for them are summarized in **Table S1**.

**Table S1** Crystal and structure refinement data for **1**.

| | |
|---|---|
| Empirical formula | $C_6H_{24}B_5N_2O_{15.5}Zn_4$ |
| Formula weight | 687.80 |
| Crystal system | Monoclinic |
| space group | *C*2/*c* |
| T/K | 293 |
| λ/Å | 1.54178 |
| *a*/Å | 26.8486(6) |
| *b*/Å | 9.8558(2) |
| *c*/Å | 17.0824(4) |
| *β*/° | 107.816(2) |
| *V*/ Å$^3$ | 4303.48(16) |
| *Z* | 8 |

| | |
|---|---|
| $D_c$/g cm$^{-3}$ | 2.123 |
| $\mu$/mm$^{-1}$ | 5.759 |
| F(000) | 2744 |
| GOF | 1.220 |
| Reflections collected | 13628 |
| Unique reflections ($R_{int}$) | 3855 (0.0205) |
| Observed reflections[$I > 2\sigma(I)$] | 3732 |
| Refined parameters | 341 |
| $R_1/wR_2$ [$I > 2\sigma(I)$] | 0.0740/0.2290 |
| $R_1/wR_2$(all data) | 0.0749/0.2295 |

## Supporting figures:

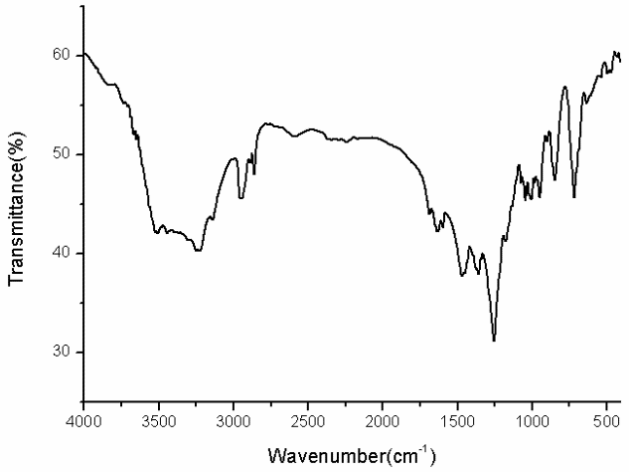


**Fig. S1** The FTIR spectrum of **1**.

As shown in **Fig. S1**, the absorption band between 3514-2861 cm$^{-1}$ are assigned as the asymmetric and symmetric stretching vibrations ofC-N, C-C, N-H, C-H, The vibrations in the region of 1633-1361cm$^{-1}$are corresponding to the bending vibrations of theN-H, C-H. The vibration absorption at 1255cm$^{-1}$is due to the B-O asymmetric bond of $BO_3$ units, whereas that of $BO_4$ units appears at 1046 and 1005cm$^{-1}$.

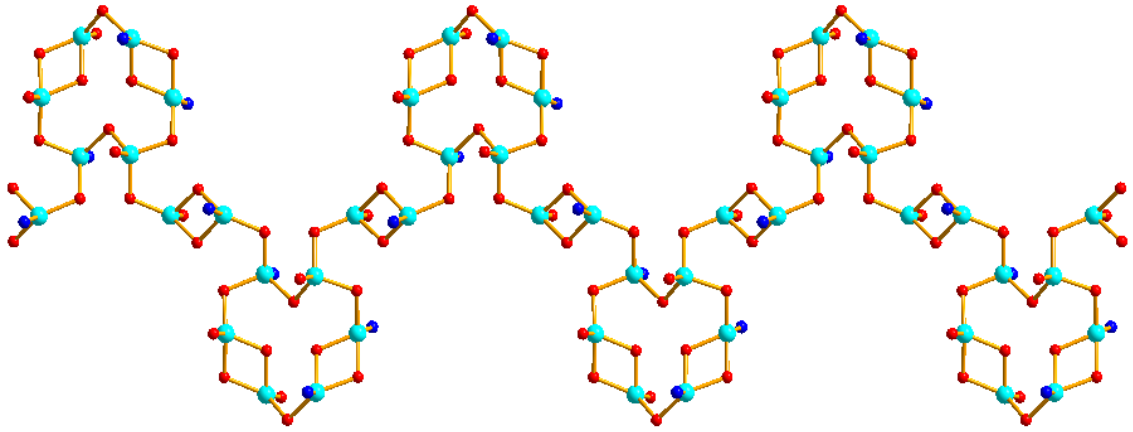

**Fig. S2** The zigzag Zn-O chain constructed from the heart-like $Zn_6O_8$ clusters and $Zn_2O_4$ dimers in the structure of **1**.

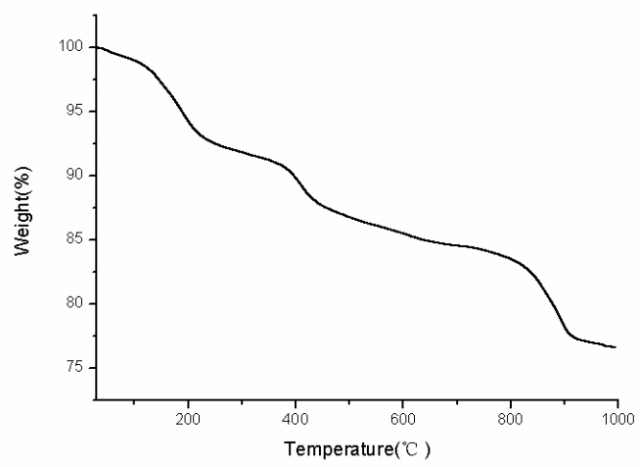


**Fig. S3** TG curve of **1**.

As shown in **Fig. S3**, TG curve of **1** shows a total weight loss of 23.43%, corresponding to the removal of water molecules, dah molecules and the successive release of the dehydration of the hydroxyls.