Electronic Supplementary Material (ESI) for Dalton Transactions.

Amino acid-templated zinc phosphites: low-dimensional structures, fluorescence, and nonlinear optical properties

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Physical measurements:

Powder X-ray diffraction (PXRD) data were obtained using a Rigaku D/MAX-rA diffractometer with Cu-Kα radiation (λ = 1.5418 Å). IR spectra (KBr pellets) were recorded on a Nicolet Impact 410 FTIR spectrometer. The thermogravimetric analyses were performed on a Netzsch STA 449c analyzer in a flow of N_2 with a heating rate of 10 ºC/min. Diffuse reflectance spectra were recorded at room temperature on a Shimadzu UV-2600 UV-vis spectrophotometer in the wavelength range of 200-800 nm. $BaSO_4$ powder was used as 100% reflectance reference.The fluorescent spectrum was collected on a FS5 Spectrofluorometer (Edinburgh instruments) equipped with a 150 W CW Ozone-free xenon arc lamp. Single crystal X-ray diffraction data were collected on a New Gemini, Dual, Cu at zero, EosS2 diffractometer at room temperature. The crystal structures were solved by direct methods. The structures were refined on F^2 by full-matrix least-squares methods using the *SHELXTL* program package.[1]

Theoretical Calculations:

The first principles calculations for $Zn(HPO_3)(C_3H_7NO_2)$ were carried out using the CASTEP suite of program to understand the relationship between structures and properties of it.[2] The band structures, density of states (DOS)/partial DOS (PDOS) and Electron-density difference (EDD) were calculated by Materials Studio (MS), under the Norm conserving pseudopotentials.[3] The kinetic cutoff energy set as 830 eV and the k-point [4] sampling in the Brilliouin zone was performed using 2 × 2 × 5. The Perdew-Burke-Ernzerhof (PBE) functional with generalized gradient approximation (GGA) was adopted for all calculations.[5] The rest parameters used in the calculations were set by the default values of the CASTEP.

Reference

1. G. M. Sheldrick, *Acta Cryst., Sect. A*, 2008, **64**, 112.

2. P. E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953.

3. K. Kobayashi, *Comp. Mater. Sci.*, 1999, **14**, 72.

4. H. J. Monkhorst and J. D. Pack, *Phys. Rev. B*, 1976, **13**, 5188.

5. D. Vanderhilt, *Phys. Rev. B*, 1990, **15**, 7892.

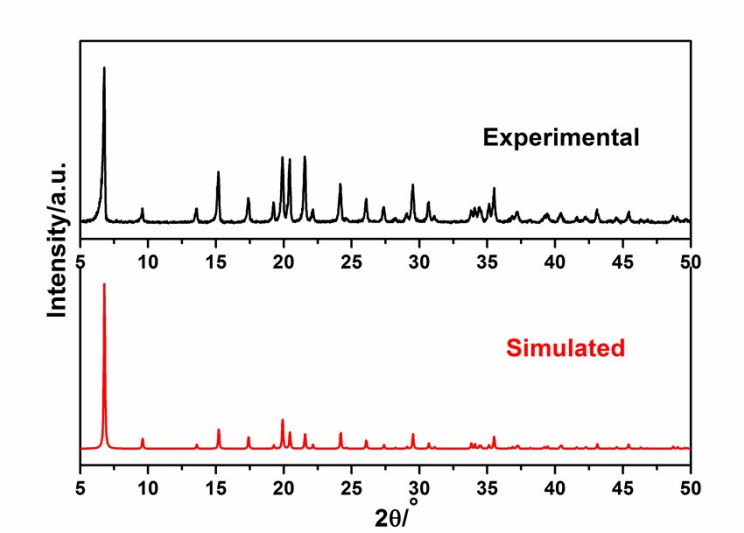

Fig. S1. Experimental and simulated PXRD patterns of SCU-6.

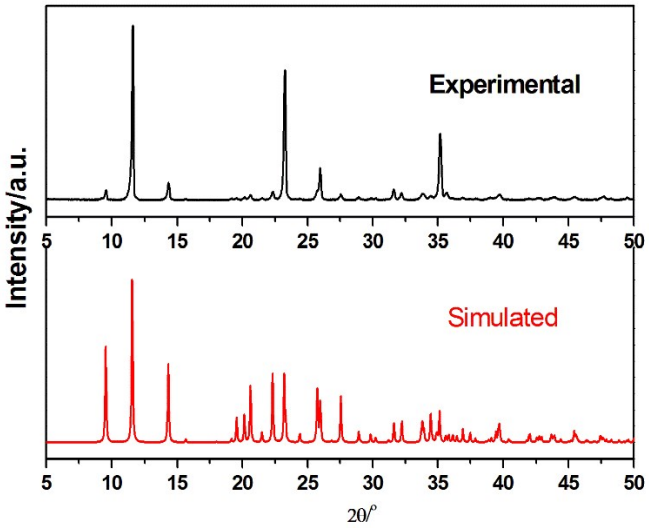

Fig. S2. Experimental and simulated PXRD patterns of SCU-15.

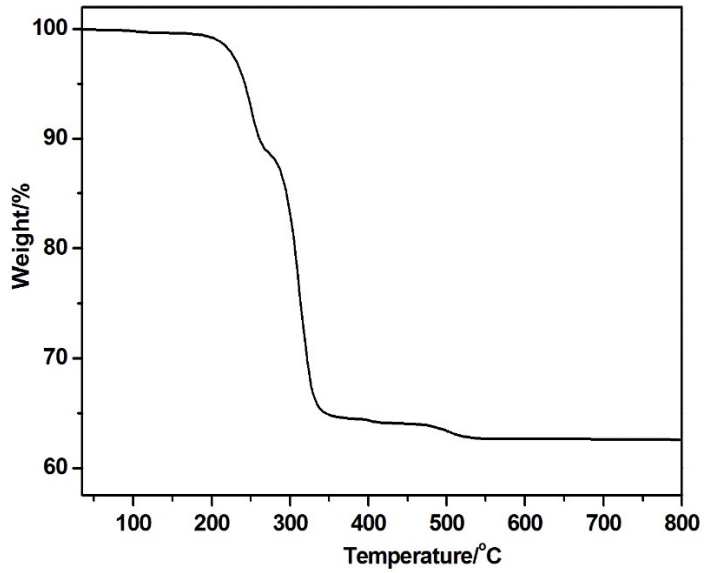

Fig. S3. The TGA curve of SCU-6.

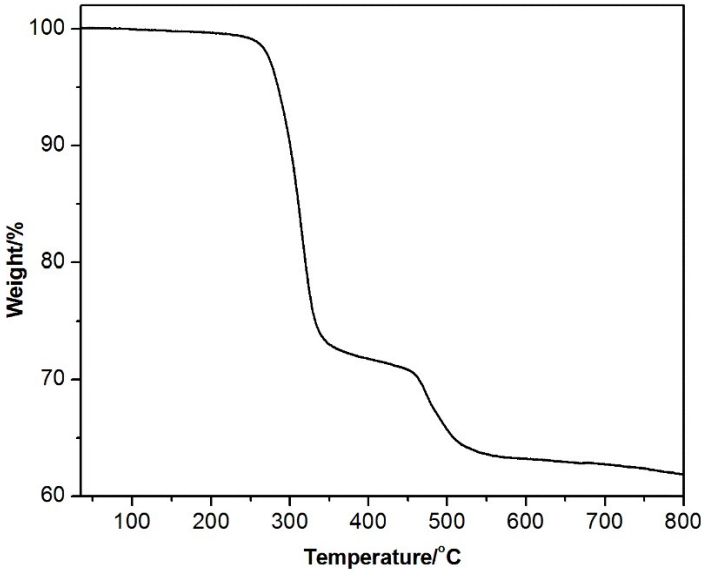

Fig. S4. The TGA curve of SCU-15.

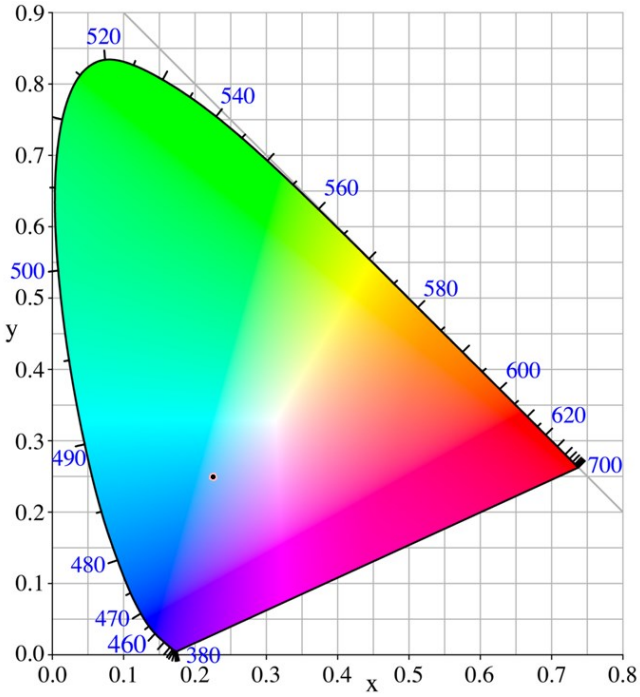

Fig. S5. The CIE coordinates for the powder sample of SCU-6.

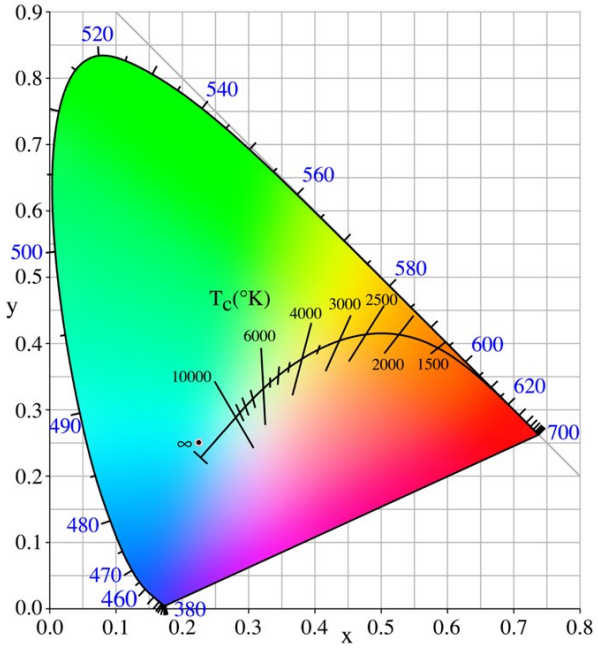

Fig. S6. The CIE coordinates for the powder sample of SCU-15.

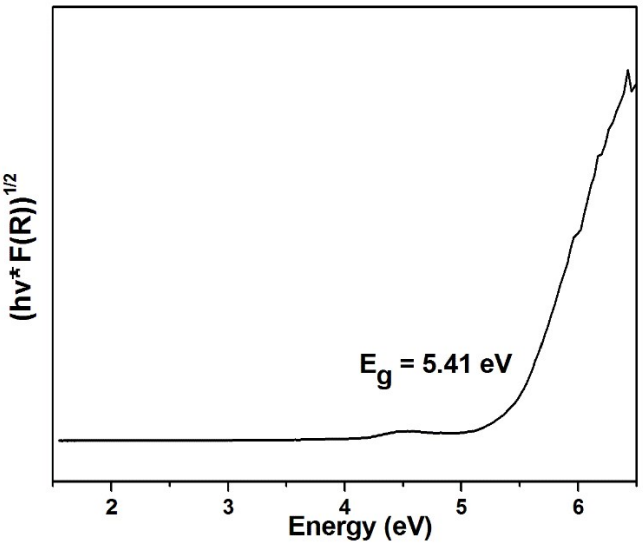

Fig. S7. Solid-state UV-vis diffuse reflectance spectrum of SCU-6.

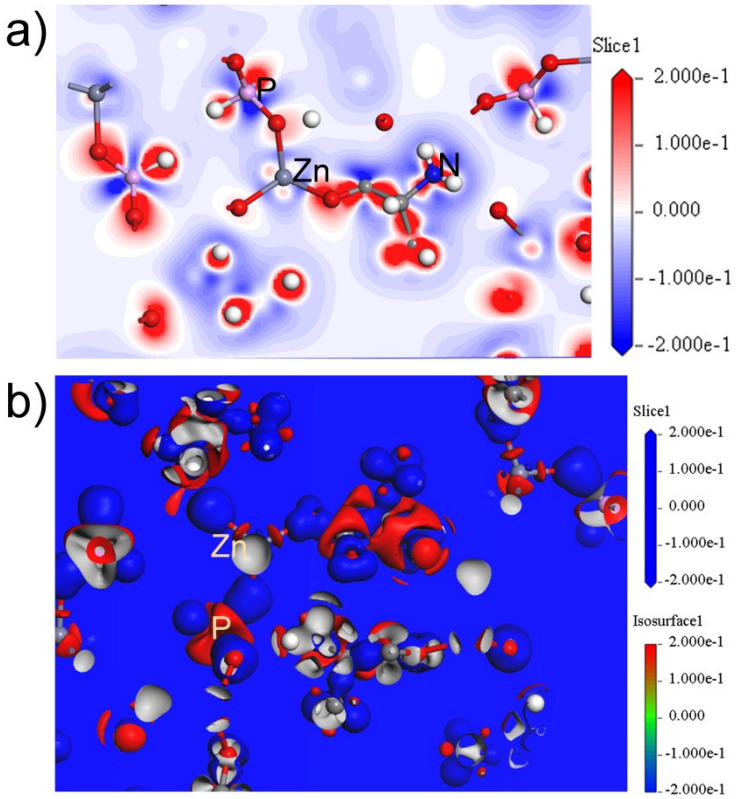

Fig. S8 (a) and (b) Electron-density difference maps of SCU-6.

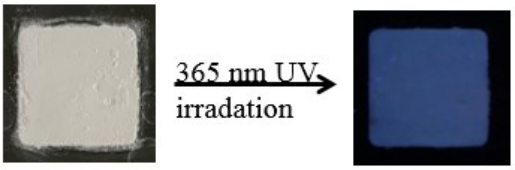

Fig. S9. Photos of SCU-6 under exposure of portable UV lamp.

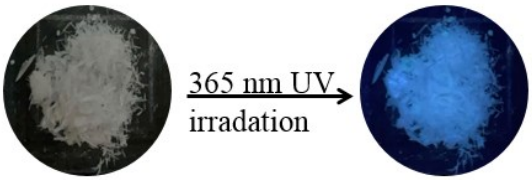

Fig. S10. Photos of SCU-15 under exposure of portable UV lamp.

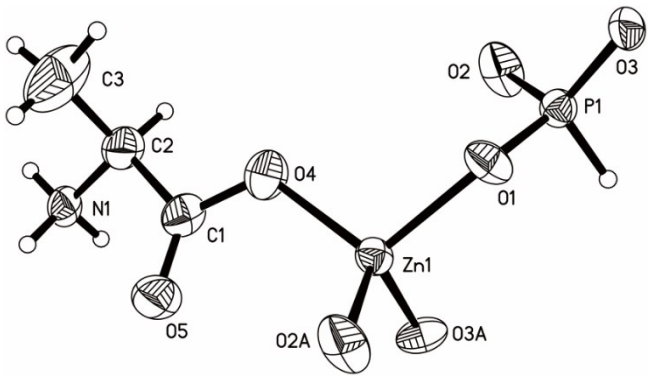

Fig. S11. ORTEP plot of the asymmetric unit of SCU-6L, showing the labeling scheme and the 50 % probability displacement ellipsoid.

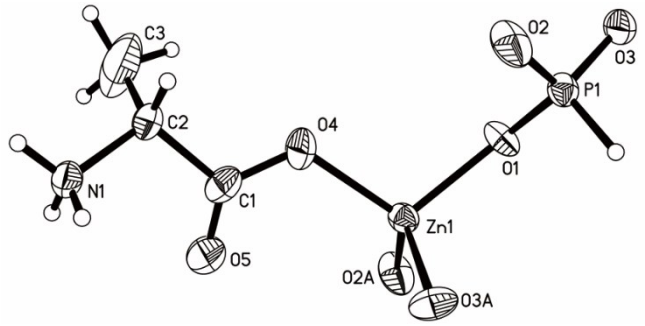

Fig. S12. ORTEP plot of the asymmetric unit of SCU-6D, showing the labeling scheme and the 50 % probability displacement ellipsoid.

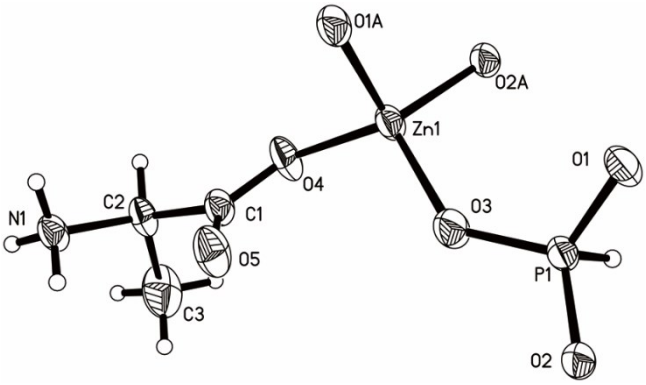

Fig. S13. ORTEP plot of the asymmetric unit of SCU-15, showing the labeling scheme and the 50 % probability displacement ellipsoid.

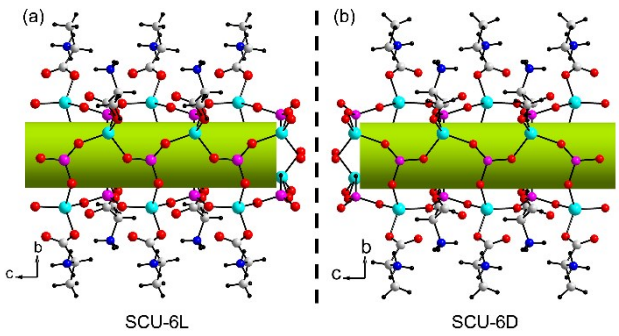

Fig. S14. Ball-and-stick representation the chiral structures of SCU-6L and SCU-6D with opposite handedness.