## Supplementary Information

## Truncated octahedral coordination cage incorporating six tetranuclearmetal building blocks and twelve linear edges †

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Fig. **S1** The truncated octahedron possessing eight trigonal ports at its faces. And six of them are plugged by the six adjacent nanospheres.



Fig. S2 Eight nanospheres inhabit at the corner of the cell view from different directions (a) viewing along [1 -3 1] direction; (b) viewing along [1 1 1] direction. The pairs in parallel with the  $C_3$  symmetry axis (namely, [1 1 1] direction) of the cell have the same polarity.



Fig. S3 Extended structure of complex 1 showing self-assembly into a layer array with ABAB<sup>...</sup> mode viewing along [1 1 1] direction.



**Fig. S4** TG-MS curves of complex **1**. The TG curve of complex **1** has one weight loss (27.3%) in the temperature range of 30-180 °C, and reaches a plateau until 415 °C before the decomposition reaction takes place. The observed species (m/z: 18, 32, 45, 46 and 87) show strong flux signals in the MS spectra when the temperature rises, which can be assigned to H<sub>2</sub>O, CH<sub>3</sub>OH, dma, Hdma<sup>+</sup> and DMA, respectively. The results indicated that the counter cations for the anionic coordination cages would be Hdma<sup>+</sup>.



Fig. S5 The hysteresis loop measured at 2 K in the -60 - 60 kOe range.



Fig. **S6** (a) The FC and ZFC curves of complex **1** with an applied field of 500 Oe. (b) The in-phase  $\chi_{m'}$  and out-of-phase  $\chi_{m''}$  components of the ac susceptibility of complex **1** measured at different frequencies (311, 911, 2911 Hz) in a zero applied dc field and an ac field of 3 Oe.



Fig. S7 PXRD of complex 1.