A large, X-shaped polyoxometalate $[As_6Fe_7Mo_{22}O_{98}]^{25-}$ assembled from $[AsMo_7O_{27}]^{9-}$ and $[FeMo_4O_{19}]^{11-}$ moieties

Panfeng Wu, Yanping Zhang, Caiting Feng, Bin Liu, Huaiming Hu and Ganglin Xue*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry (Ministry of Education), Department of Chemistry, Northwest University, Xi'an, 710069, China

E-mail: xglin707@163.com

Magnetic measurements: Magnetic susceptibility measurements were performed on previously ground, hand-collected crystals (9.73 mg, restrained in eicosane to prevent torquing at high fields) with a Quantum Design MPMS-XL-7 magnetometer. The susceptibility data were corrected from the diamagnetic contributions as deduced by using Pascal's constant tables. Direct current (dc) data were collected in the range of 1.8-300 K with an applied field of 1000 G. Thermogravimetric analysis was performed on a NETZSCH STA 449C TGA instrument in flowing N_2 with a heating rate of 10 °C·min^{-1}. IR spectra were recorded in the range of 400-4000 cm^{-1} on an EQUINOX55 FT/IR spectrophotometer using KBr pellets. The powder X-ray diffraction (PXRD) data were collected on a Bruker D8 diffractometer with Cu Kα radiation.

Fig. S1 ball-and-stick representation for $[As_6Fe_7Mo_{22}O_{98}]^{25-}$

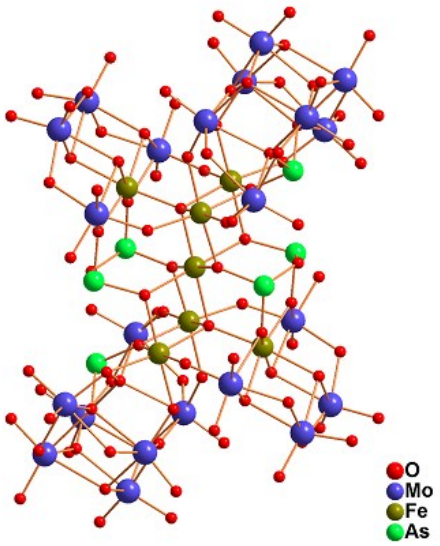

Fig. S2 IR spectra for $(NH_4)_{25}[As_6Fe_7Mo_{22}O_{98}]\cdot 13H_2O$

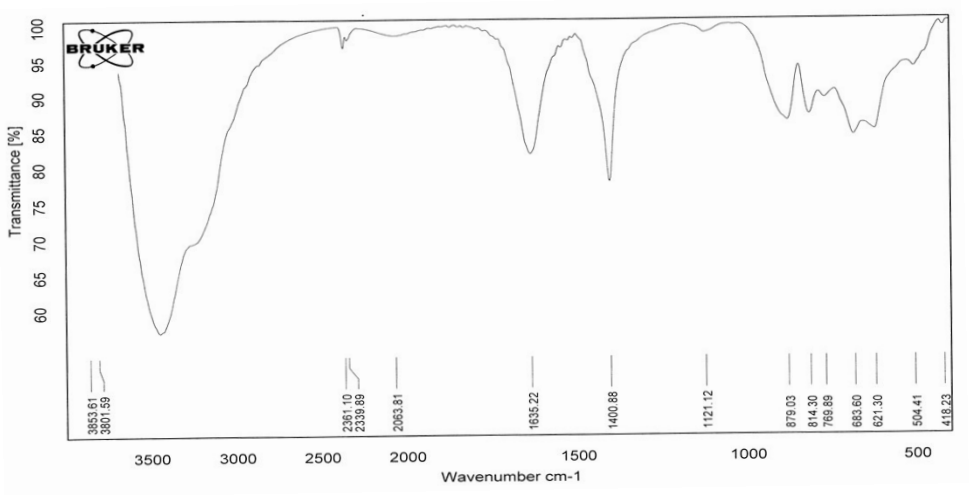

Fig. S3 Comparison of the simulated and experimental XRD patterns of $(NH_4)_{25}[As_6Fe_7Mo_{22}O_{98}]\cdot 13H_2O$

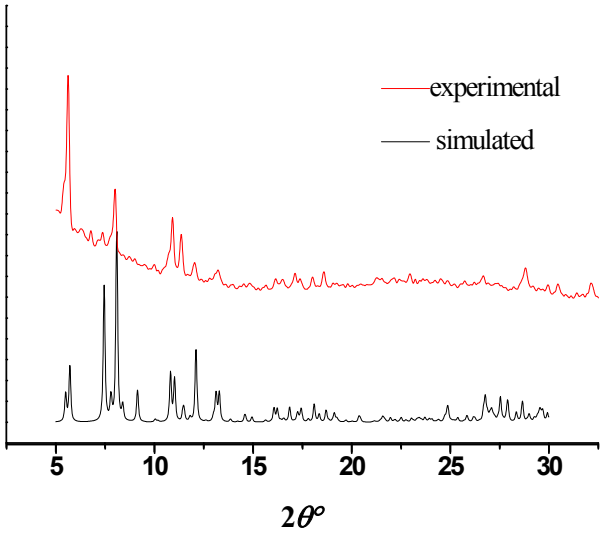

Fig. S4 TG curve of $(NH_4)_{25}[As_6Fe_7Mo_{22}O_{98}]\cdot 13H_2O$

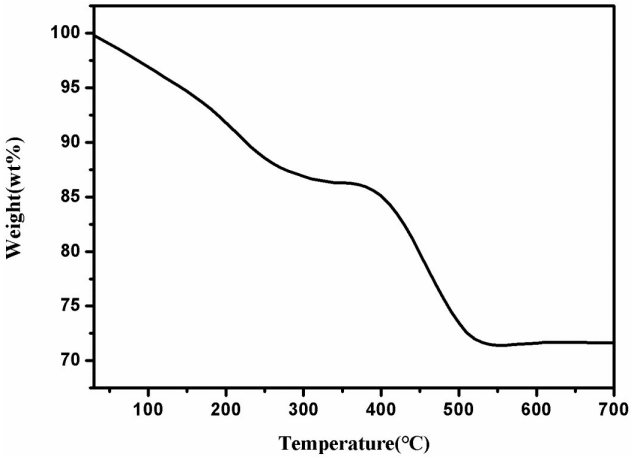

Table S1. Bond valence sum values for As, Fe and W atoms in **1**.

atoms	BVS value	atoms	BVS value
Fe1	2.93	Mo6	6.00
Fe2	2.94	Mo7	6.11
Fe3	2.78	Mo8	6.00
Fe4	2.92	Mo9	6.17
Mo1	5.99	Mo10	5.96
Mo2	5.96	Mo11	6.03
Mo3	6.05	As1	2.94
Mo4	5.90	As2	3.03
Mo5	6.05	As3	3.10