Electronic Supplementary Information for Dalton Transactions

Supplementary Materials

Two new cantilever-type polyoxometalates constructed from $\{Mo_2O_4\}^{2+}$ fragments and diphosphonates

Huaqiao Tan,[a] Weilin Chen,[a] Ding Liu,[a] Yangguang Li*,[a] and Enbo Wang*,[a]

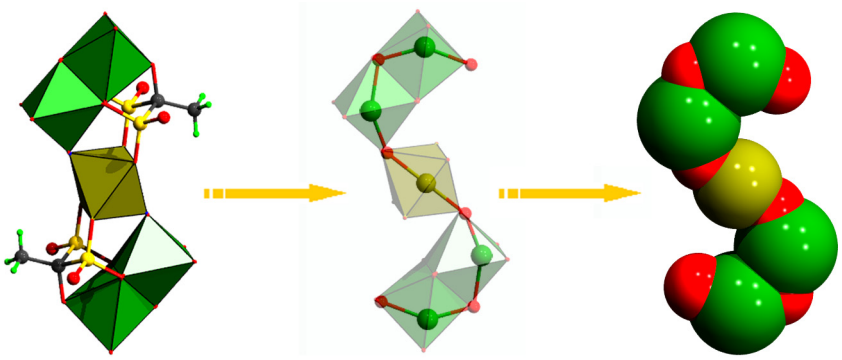


Figure S1. The "S"-shaped structure of polyoxoanion **1** constructed by MoO_6 and VO_6 octahedra.

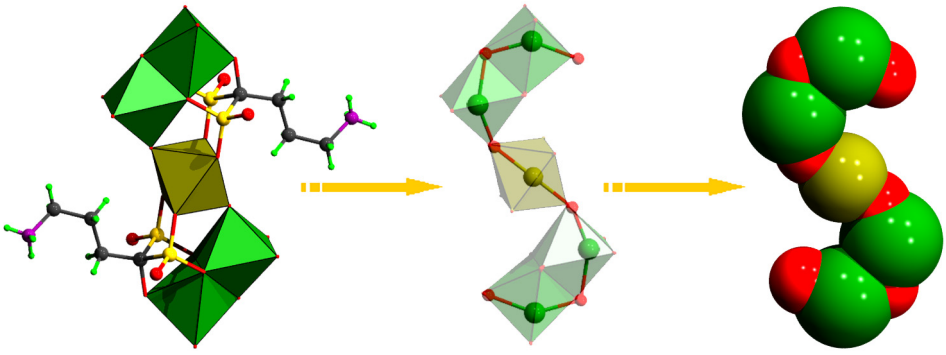


Figure S2. The "S"-shaped structure of polyoxoanion **2** constructed by MoO_6 and VO_6 octahedra.

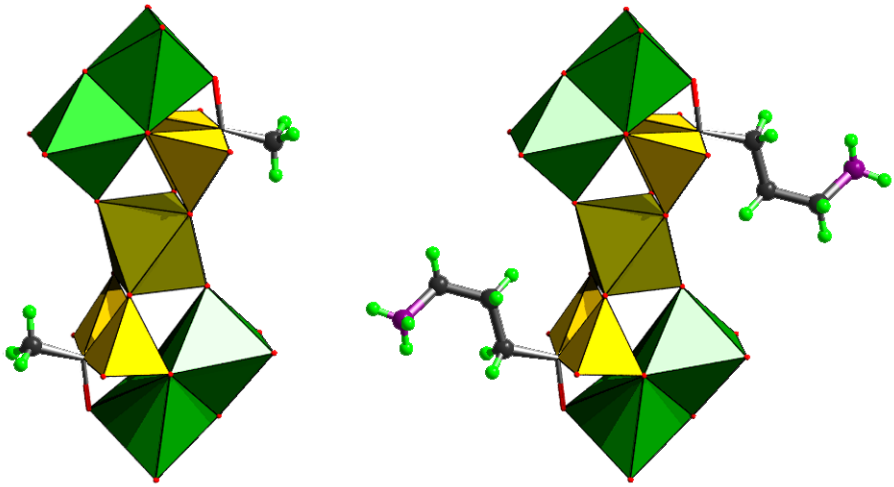


Figure S3. Polyhedral and ball-and-stick representation of the cantilever-type structure of polyoxoanion **1** (a) and **2** (b).

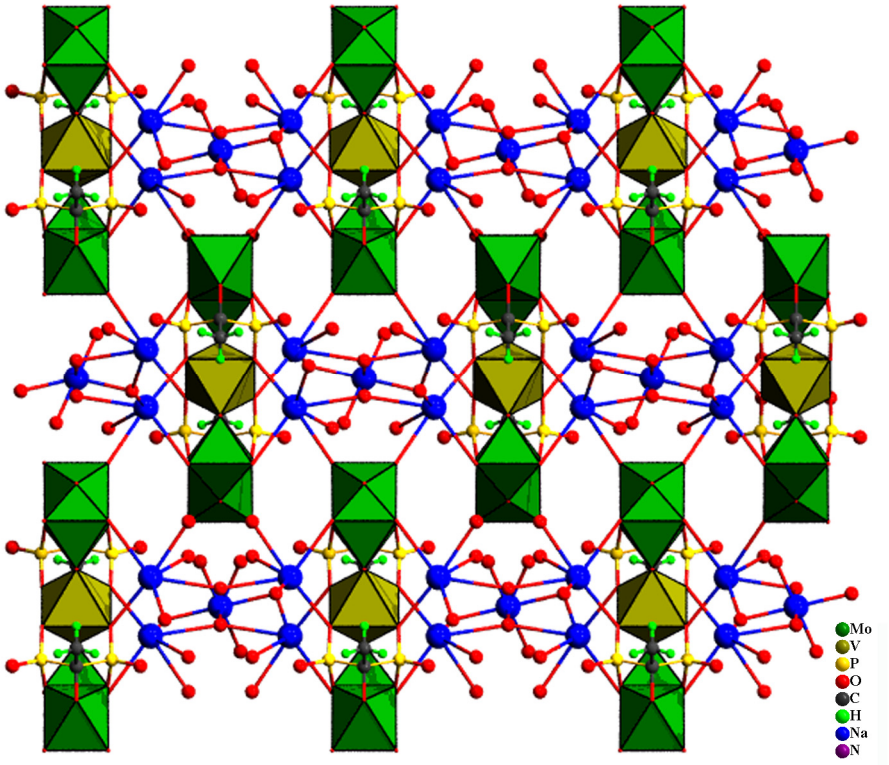


Figure S4. Polyhedral and ball-and-stick representation of the 3D structure of polyoxoanion **1** connected by Na^{+} viewed from a axis.

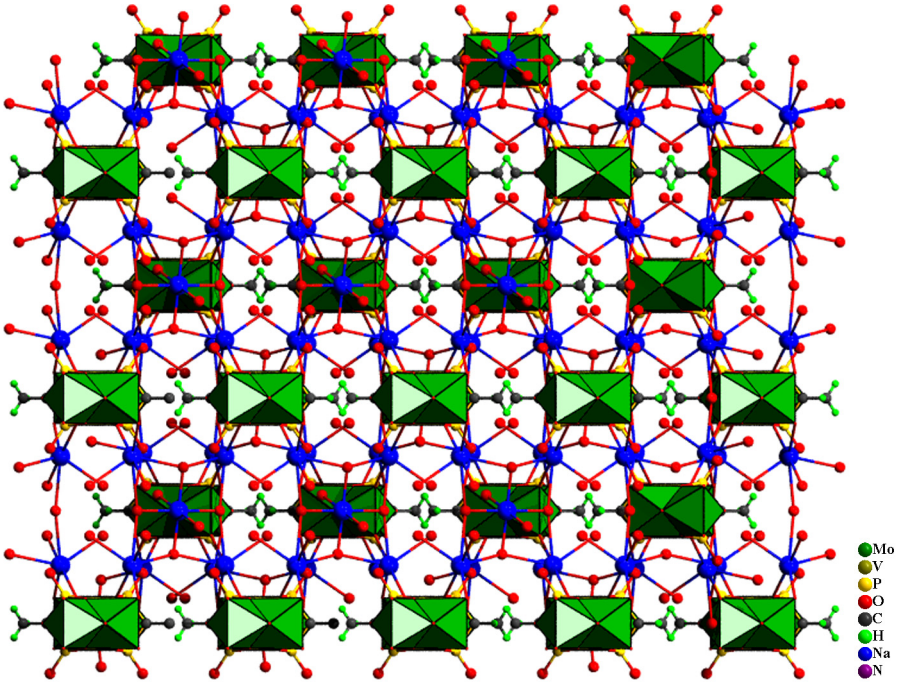


Figure S5. Polyhedral and ball-and-stick representation of the 3D structure of polyoxoanion **1** connected by Na^+ viewed from b axis.

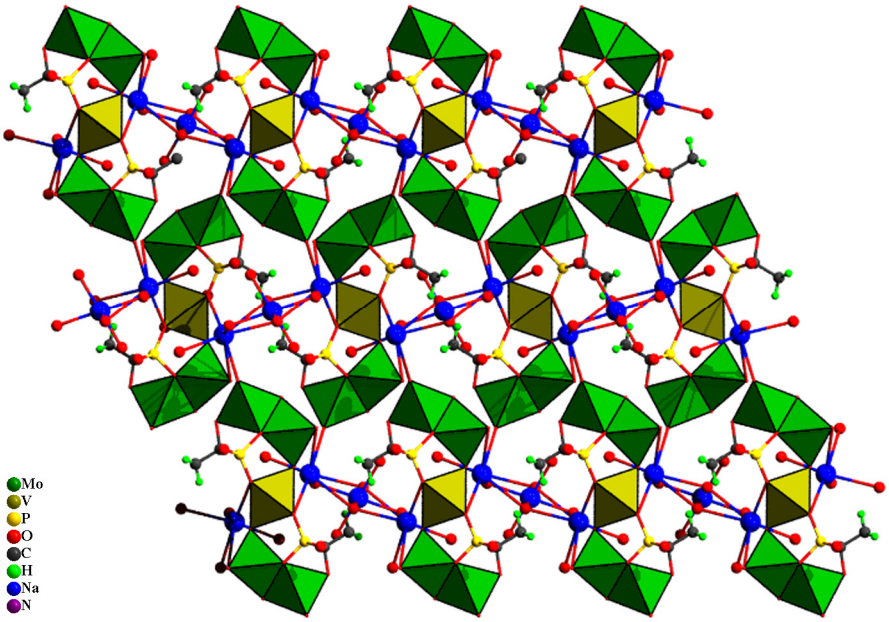


Figure S6. Polyhedral and ball-and-stick representation of the 3D structure of polyoxoanion **1** connected by Na^+ viewed from c axis.

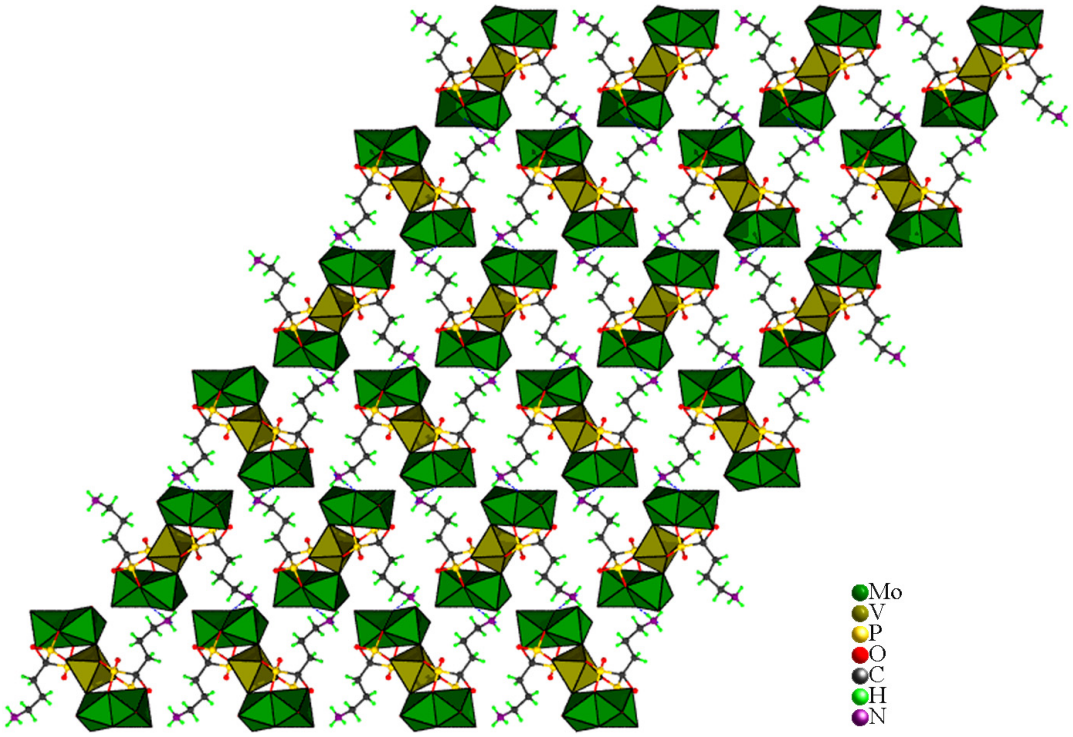


Figure S7. Polyhedral and ball-and-stick representation of 3D supramolecular framework in compound **2** viewed from a axis.

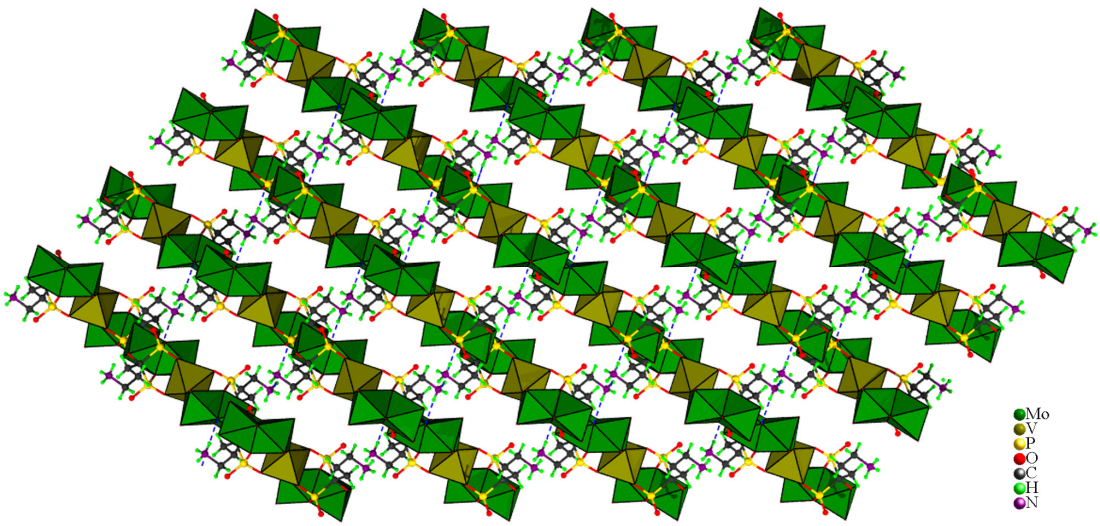


Figure S8. Polyhedral and ball-and-stick representation of 3D supramolecular framework in compound **2** viewed from b axis.

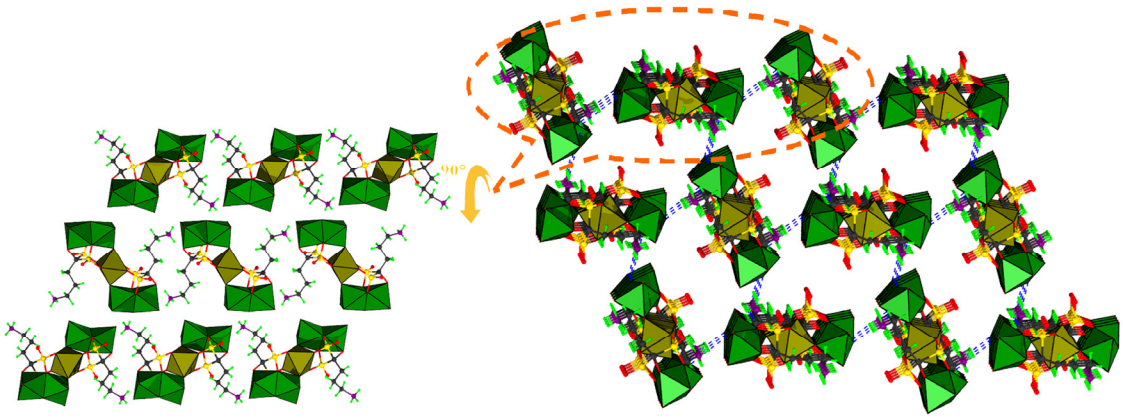


Figure S9. Polyhedral and ball-and-stick representation of 3D supramolecular framework in compound **2** viewed from c axis.

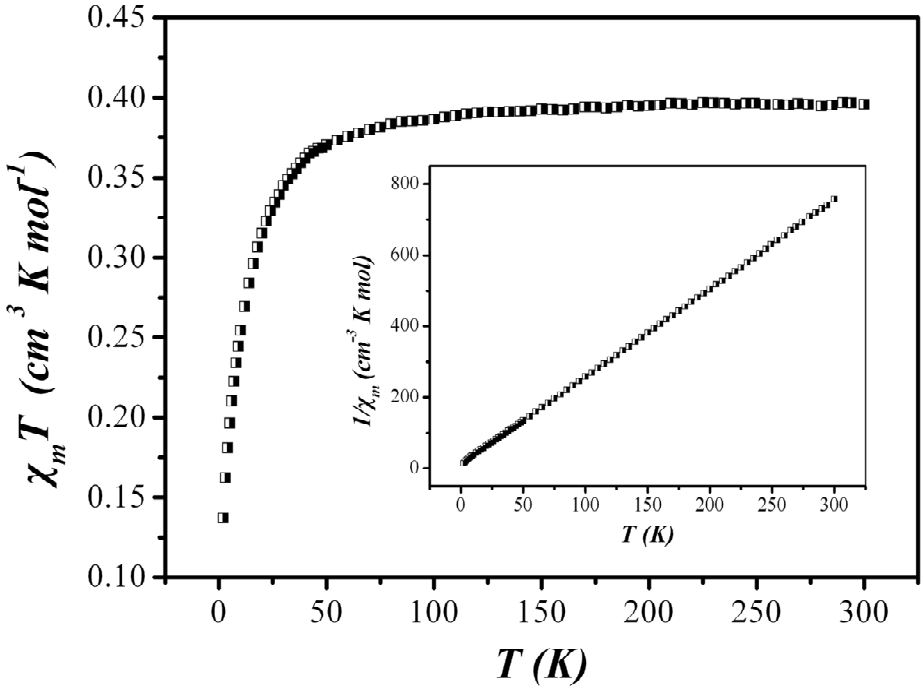
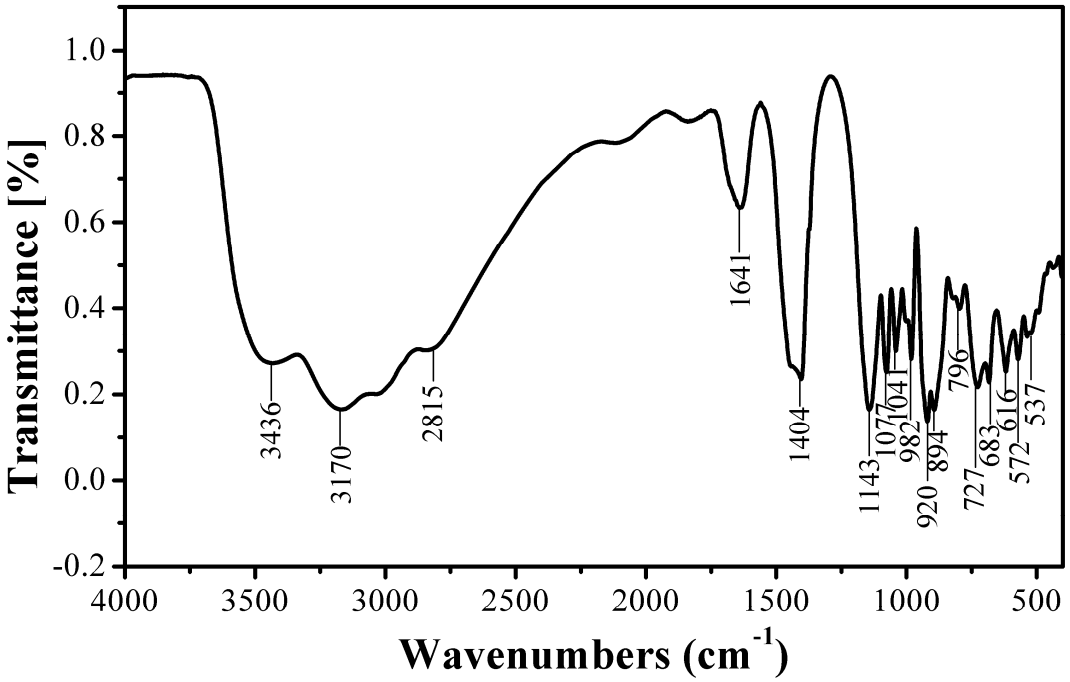


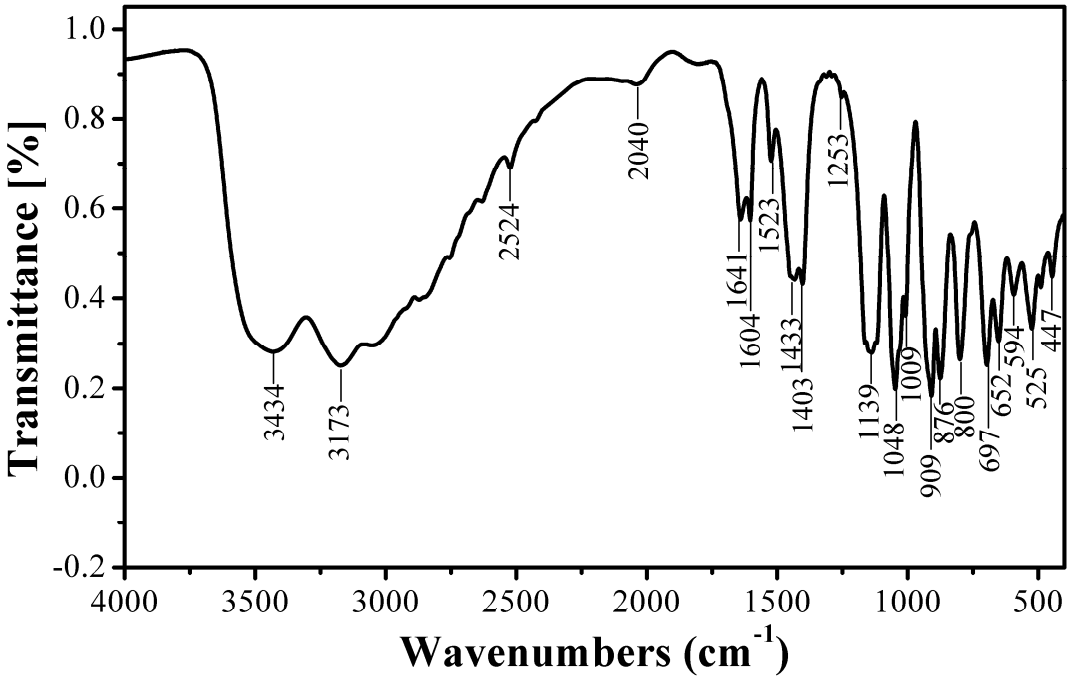
Figure S10. Thermal variation of χT and χ-1 for compound **2.**

Magnetic studies has been performed on the powdered sample of **2** in the range of 2–300 K. The temperature dependence of the magnetization was studied in a 1000 Oe field. Figure. 10S shows the magnetic behavior of **2** in the form of χT versus T and χ^{-1} versus T plots (where χ is the molar magnetic susceptibility). Upon cooling, the χT continuously decreases, indicating the presence of the antiferromagnetic interactions. The χT value for **2** is 0.396 $cm^3 \cdot K \cdot mol^{-1}$ at 300 K and 0.137 $cm^3 \cdot K \cdot mol^{-1}$ at 2K, respectively. The χT value per formular unit at 300 K is slightly higher than that expected for the total spin-only value of one uncoupled S = 1/2 spin of V^{4+} atom (χT

= 0.375 $cm^3 \cdot K \cdot mol^{-1}$). The magnetic behaviours of sample **2** obeys the Curie-Weiss law with C = 0.40 $cm^3 \cdot K \cdot mol^{-1}$ and θ = -4.84 K, being the characteristic of an overall antiferromagnetic interaction.

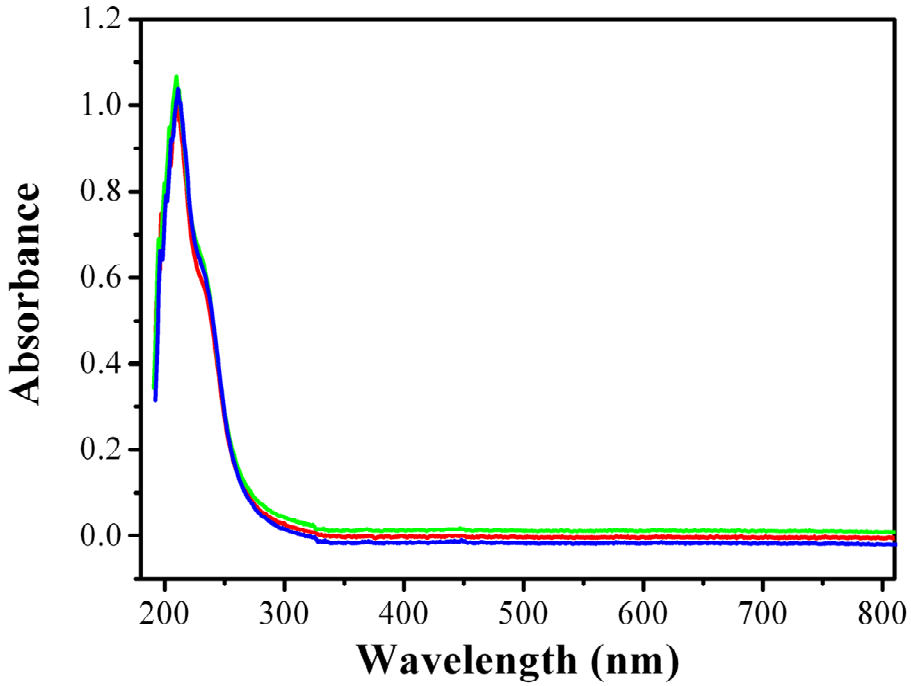


(a)



(b)

Figure S11. IR spectrum for compounds **1** (a), **2** (b).



(a)

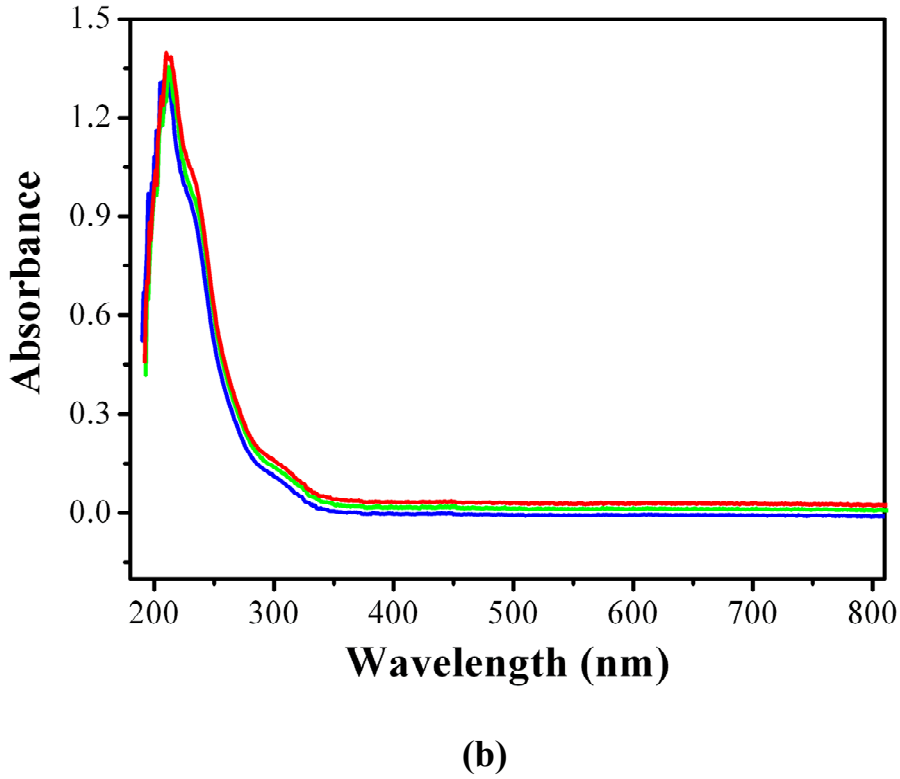


Figure S12. The UV-Vis spectrum for compounds **1** (a) and **2** (b) in aqueous solution.

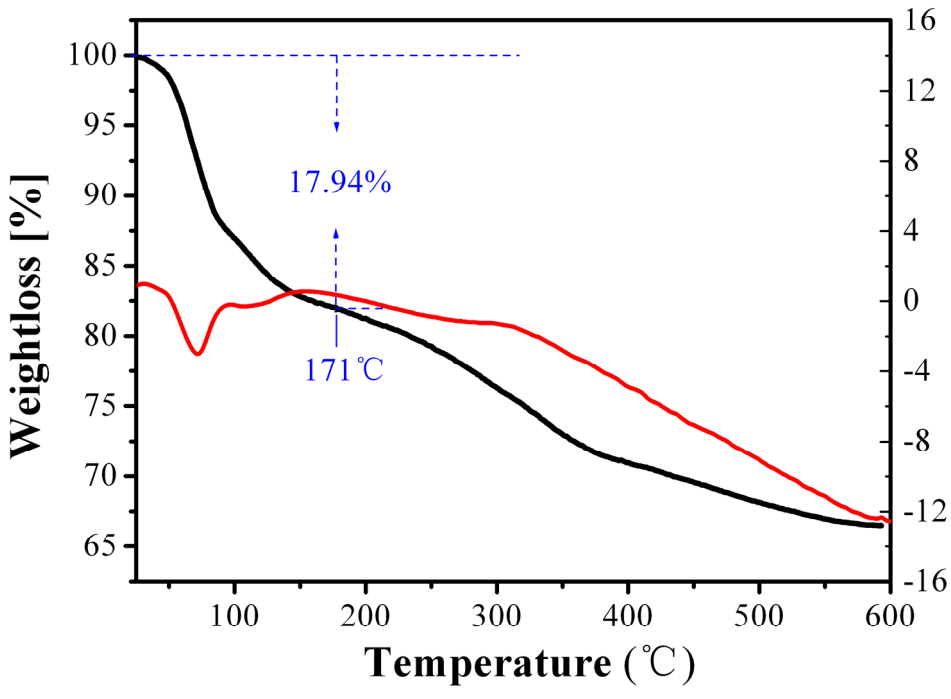


Figure S13. The TG curve of **1** exhibits two weight loss stages in the temperature ranges 20-600°C. The first weight loss is 17.95% in the temperature range 20-171°C, corresponding to the release of all the NH_4^+ ions, lattice and coordinated water molecules in **1** (18.05%). And after 171°C, polyoxoanion **1** would be decomposed.

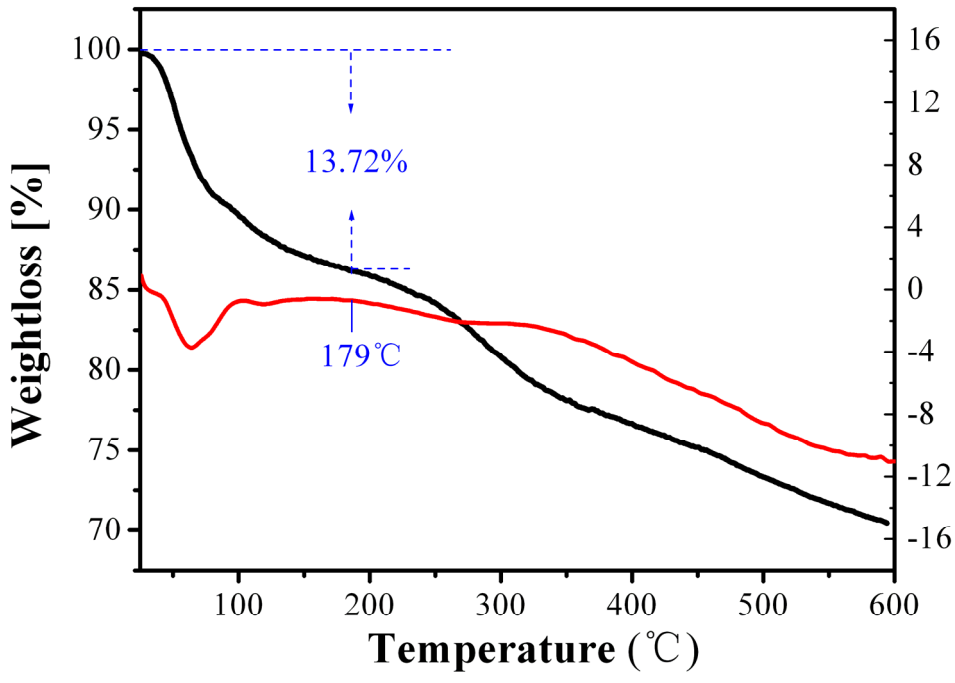
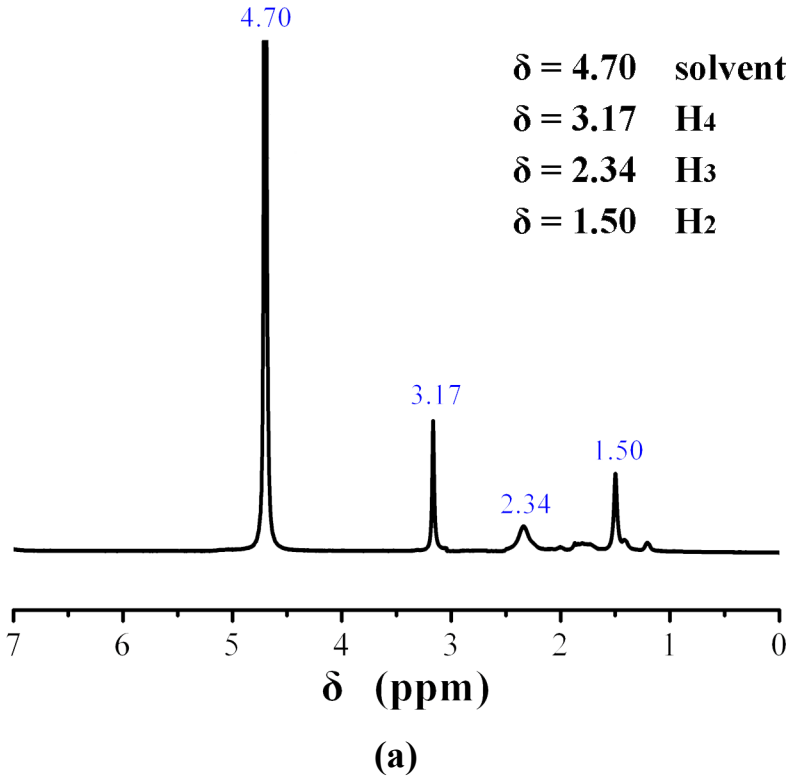
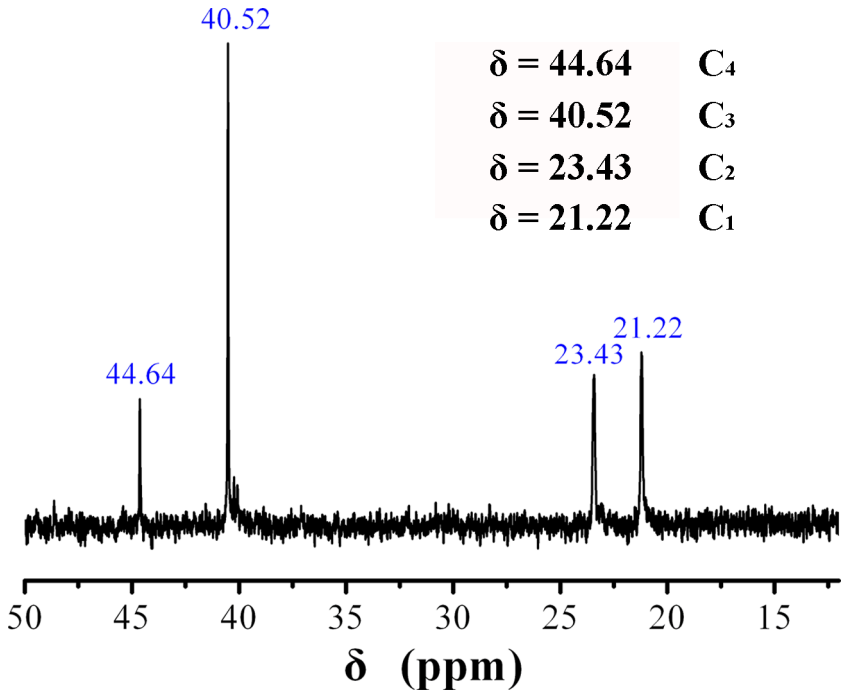


Figure S14. The TG curve of **2** exhibits two weight loss stages in the temperature ranges 20-600°C. The first weight loss is 13.72% in the temperature range 20-179°C, corresponding to the release of all the NH_4^+ ions and lattice water molecules in **2** (13.87%). And after 179°C, polyoxoanion **2** would be decomposed.



(a)



(b)

Figure S14. (a) The ^{1}H spectrum of compound **2**; (b) The ^{13}C spectrum of compound **2**.