

Supplementary Information

Figure S1

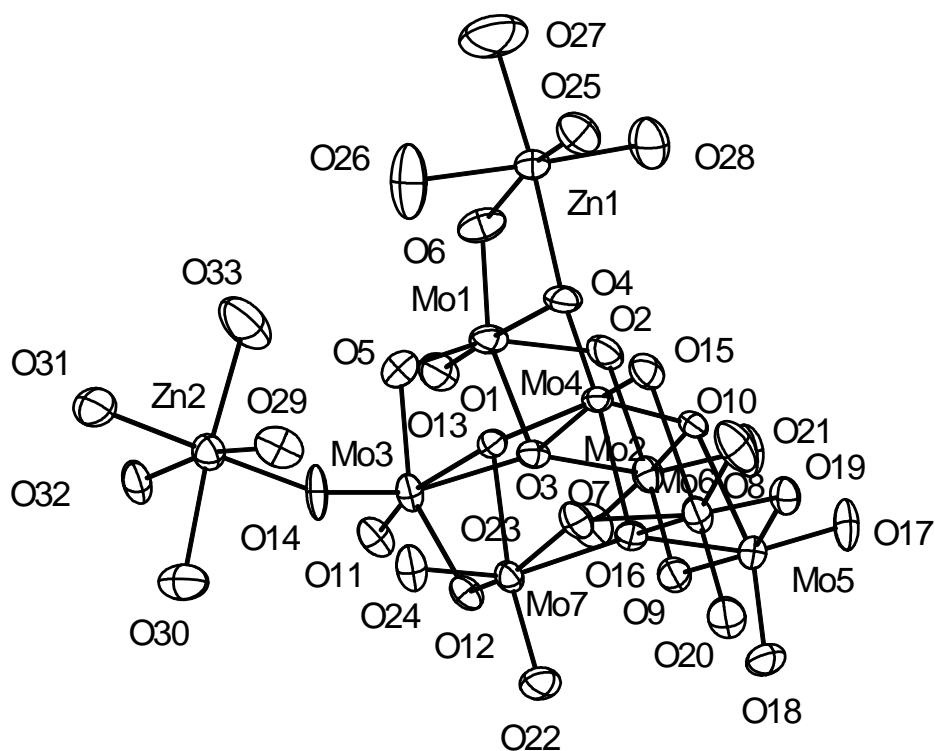


Figure S1. Thermal ellipsoidal representation of $[\{Zn(H_2O)_5\}\{Zn(H_2O)_4\}\{Mo_7O_{24}\}]^{2-}$ with 50% probability.

Figure S2

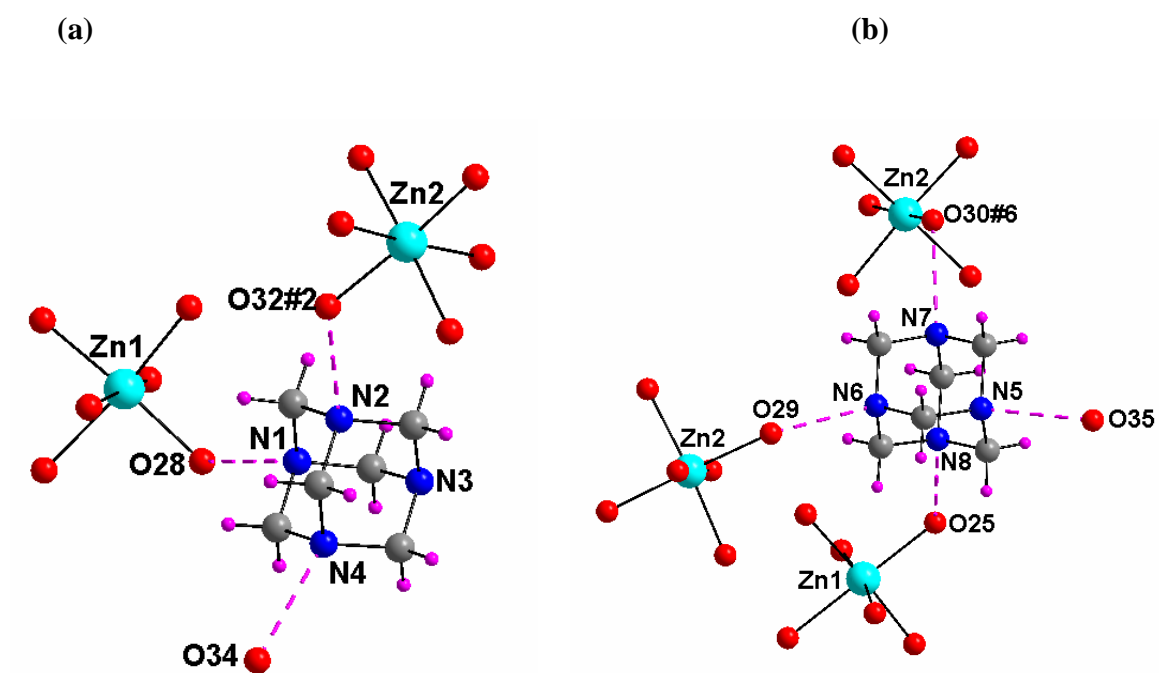


Figure S2. The Hydrogen bonding interaction of the amine cations [namely (a) ‘N1N2N3N4’ and (b) ‘N5N6N7N8’] with surrounding zinc complexes and lattice water molecules. Color code: O, red; C, gray; H, purple; Zn, cyan; N, blue; purple dotted lines represent the N–H···O / O–H···N hydrogen bonding interactions.

Figure S3

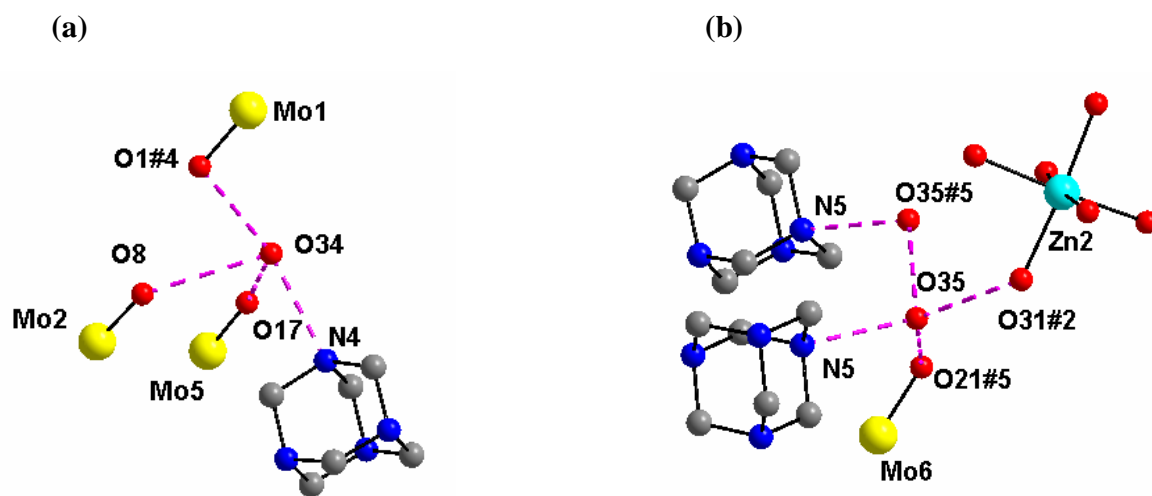


Figure S3. The hydrogen bonding situation (only N–H···O / O–H···N interaction) around the lattice water molecules (O34 and O35): (a) around O34 water molecule (b) around O35 water molecule (hydrogen atoms of organic amines are omitted for clarity). Color code: O, red; Mo, yellow; C, gray; Zn, cyan; N, blue; purple dotted lines represent the hydrogen bonding interactions.

Figure S4

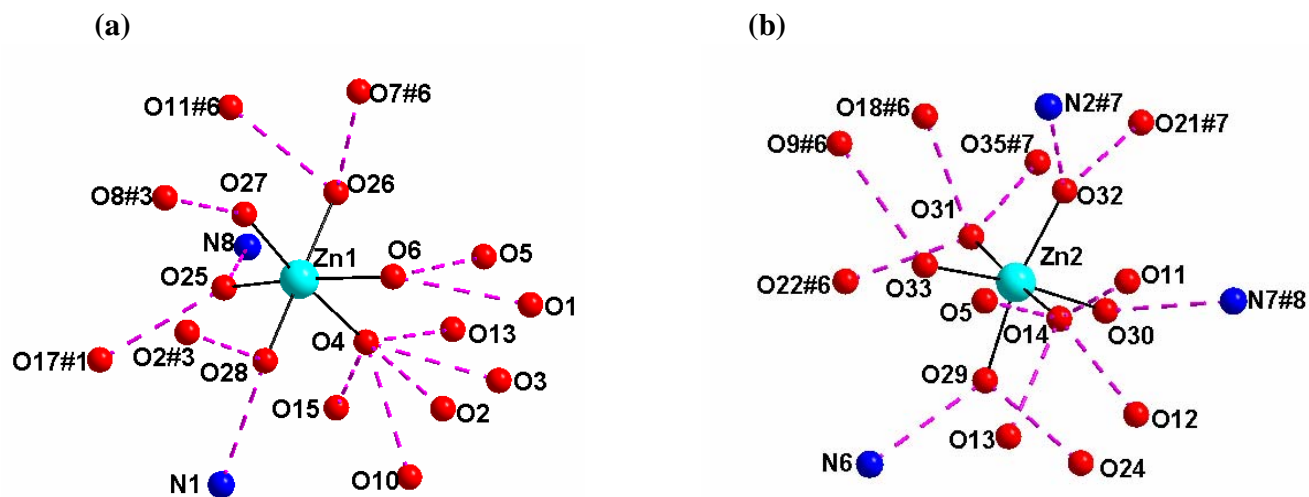


Figure S4. The weak supramolecular O–H···O and N–H···O / O–H···N hydrogen bonding interactions of Zinc complexes with surrounding heptamolybdate anion and organic amine cations resulting in a complicated hydrogen bonding situation. Color code: O, red; Zn, cyan; N, blue; purple dotted lines represent the hydrogen bonding interactions.

Figure S5

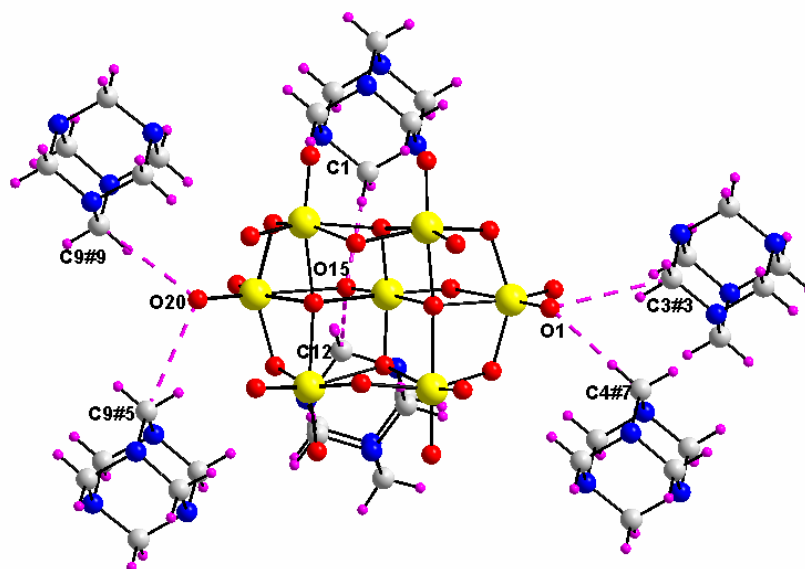
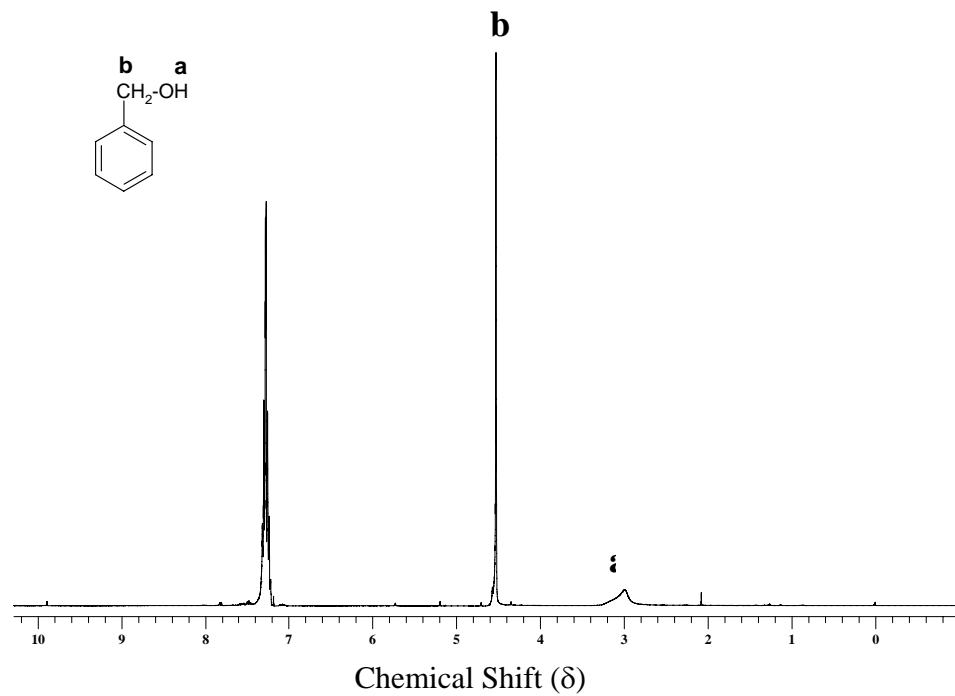


Figure S5. The C–H...O hydrogen bonding interaction of [Mo₇O₂₄]⁶⁻ anion with surrounding amine cations. Color code: O, red; Mo, yellow; C, gray; H, purple; Zn, cyan; N, blue; purple dotted lines represents the hydrogen bonding interactions.

Figure S6

(a)



(b)

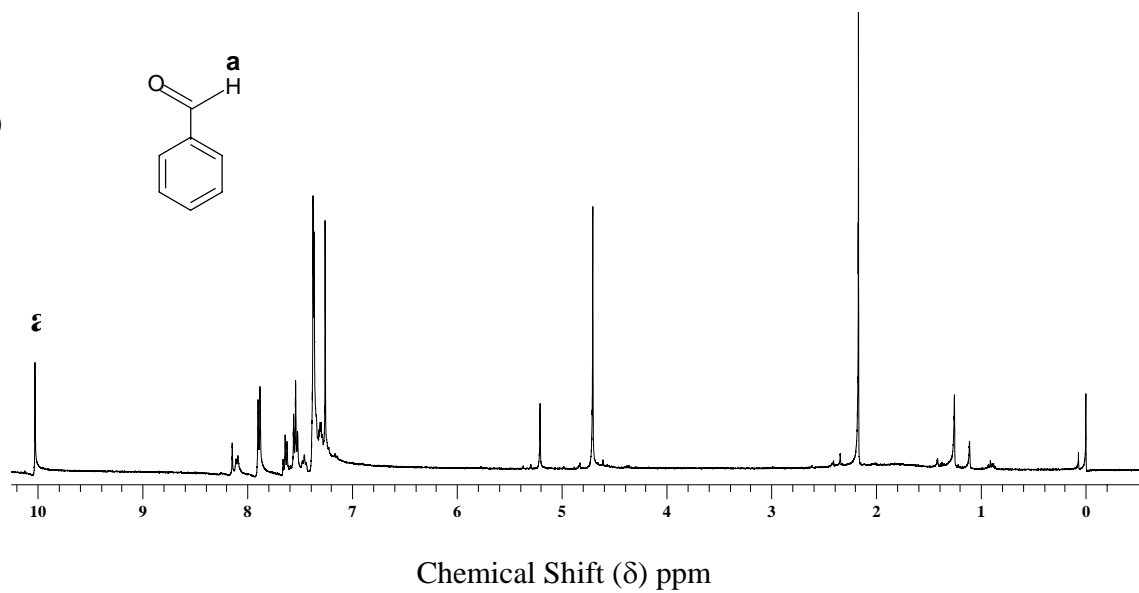


Figure S6. 400 MHz ^1H NMR spectrum of (a) distilled benzyl alcohol in CDCl_3 and (b) product mixture in CDCl_3 . ($-\text{CHO}$ peak is marked as 'a').

Figure S7

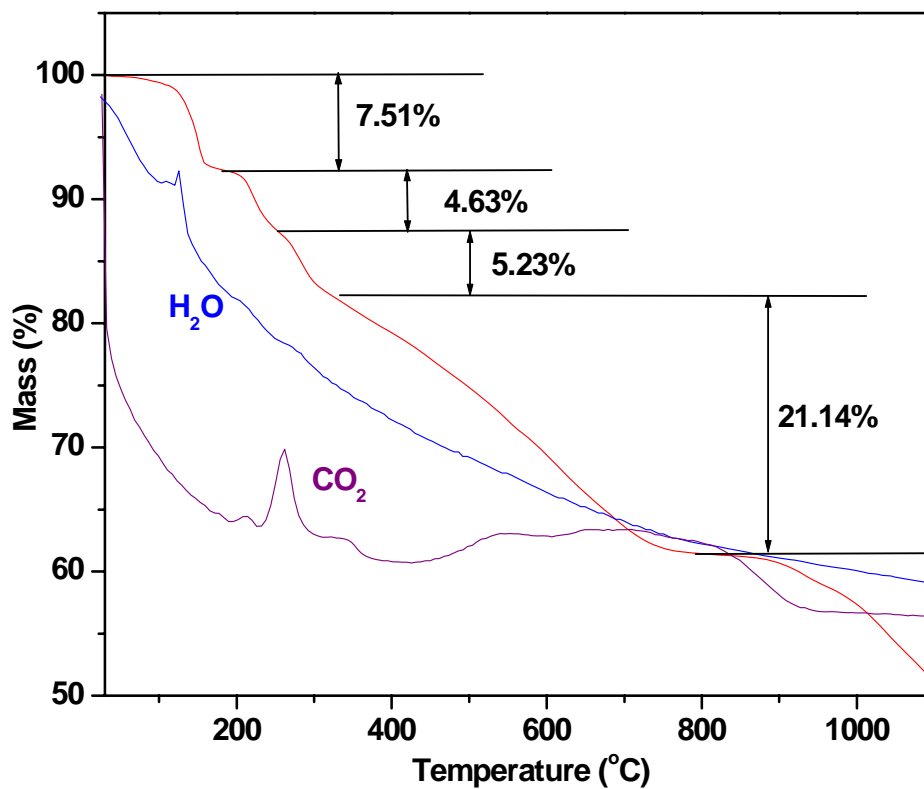


Figure S7. The TGA/Mass analysis graph for compound 1. The water and carbon dioxide mass-loss curves are represented in blue and violet color respectively.

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