

Supplementary Materials

Non-covalent O...O interactions among isopolyanions using a *cis*-{MoO₂} moiety by the assistance of N–H...O hydrogen bonds

T. Arumuganathan, A. Srinivasa Rao and Samar K. Das*

School of chemistry, University of Hyderabad, Hyderabad 500 046

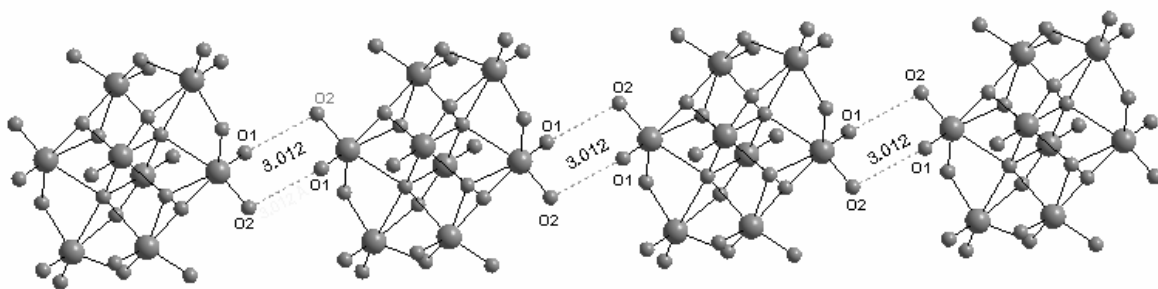


Figure S1. O...O non-covalent interactions among the isopolyanions $[\text{Mo}_8\text{O}_{26}]^{4-}$ leading to a chain like structure.

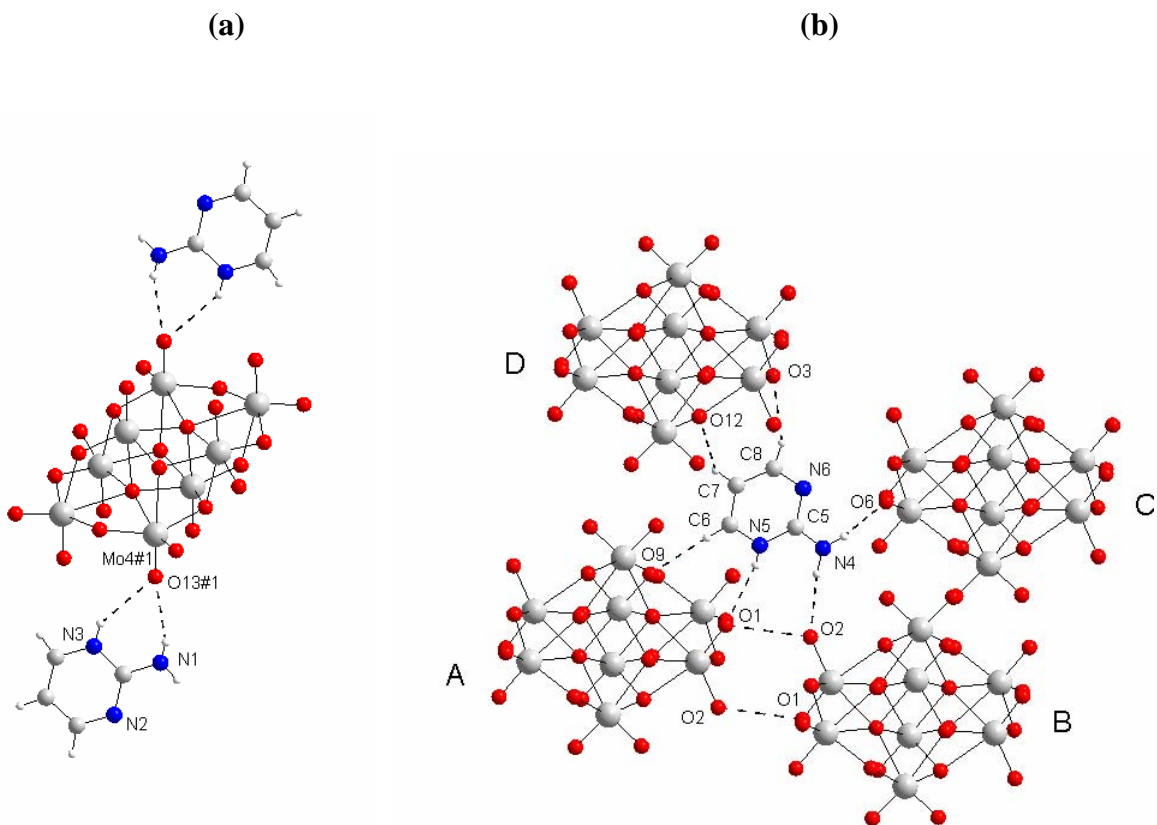


Figure S2. (a) One of the crystallographically independent organic cation namely ‘N1N2N3’ exhibiting hydrogen bonding interactions to the cluster anion in a bifurcated manner. (b) The immediate hydrogen bonding environment around ‘N4N5N6’ cation is presented.

As shown in figure S2b, interestingly, five ring atoms (C5, C6, C7, C8 and N5), out of total six ring atoms of the organic cation, is involved in hydrogen bonding interactions with its four surrounding isopolyanions, which are designated as A, B, C and D. Among these, A and B isopolyanions are the part of the chain, that is formed by O···O contacts among isopolyanions (figure S1).

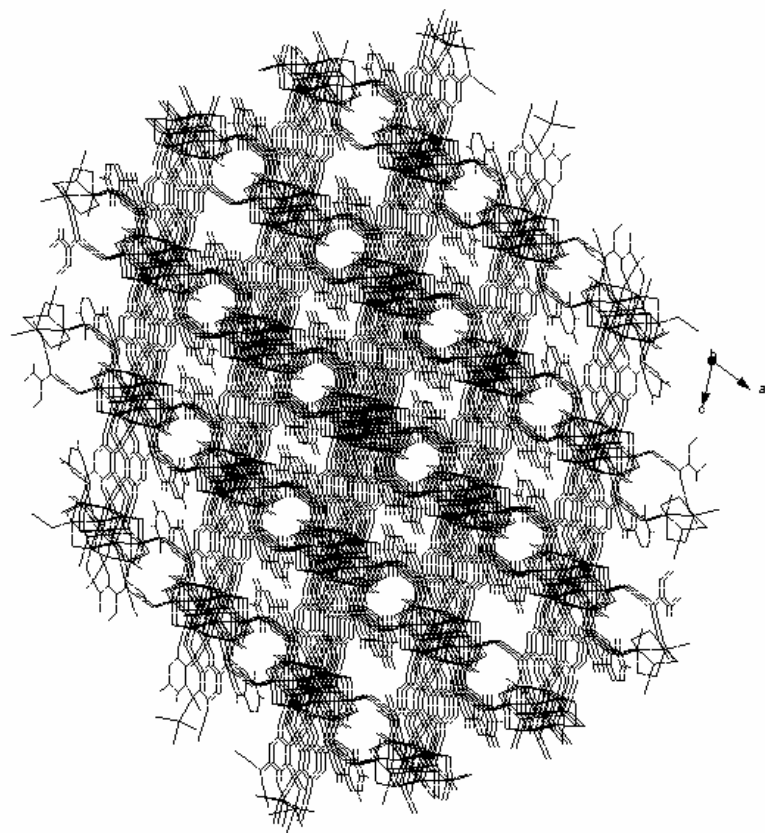


Figure S3. The Wire frame representation of the three-dimensional supramolecular structure of $[2\text{-AmpH}]_4[\text{Mo}_8\text{O}_{26}]$ (**1**) having well-defined channels.

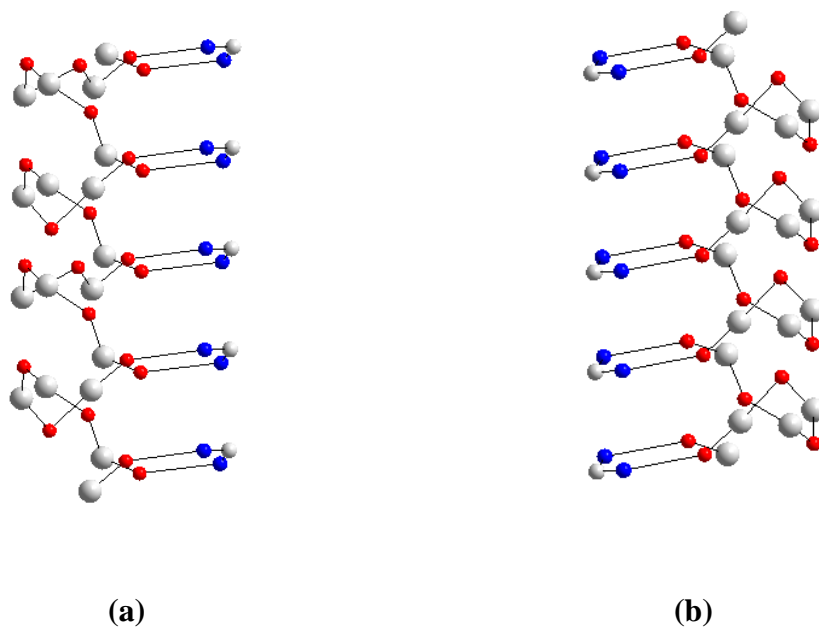


Figure S4. Helical arrangement formed from the isopolyanion and ‘N4N5N6’ organic cation: (a) the ball-and-stick model of the supramolecular left-handed helical backbone. (b) the ball-and-stick model of the supramolecular right-handed helical backbone.

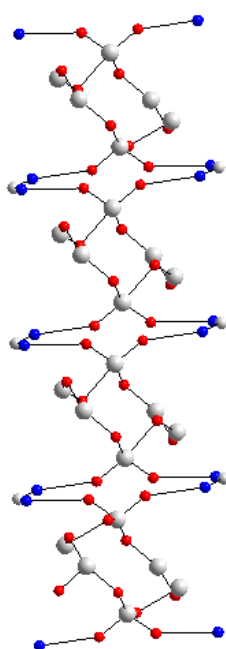


Figure S5. The double helical arrangement formed from both left- and right-handed helices (helical backbone is shown).

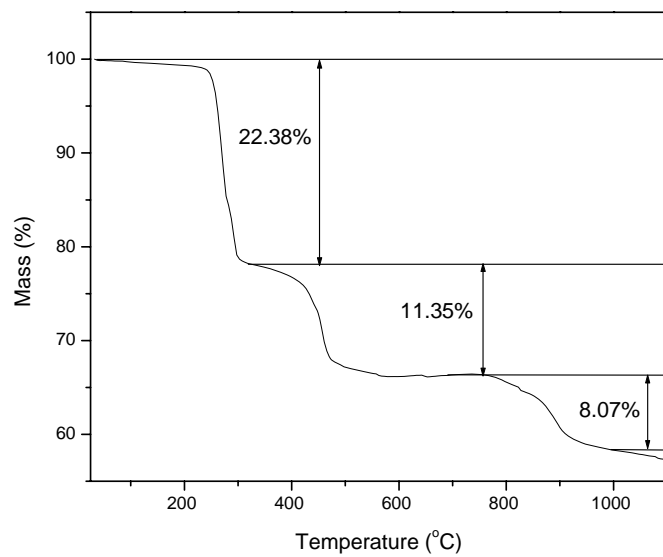


Figure S6. TGA plot of compound [2-AmpH]₄[Mo₈O₂₆] (1)

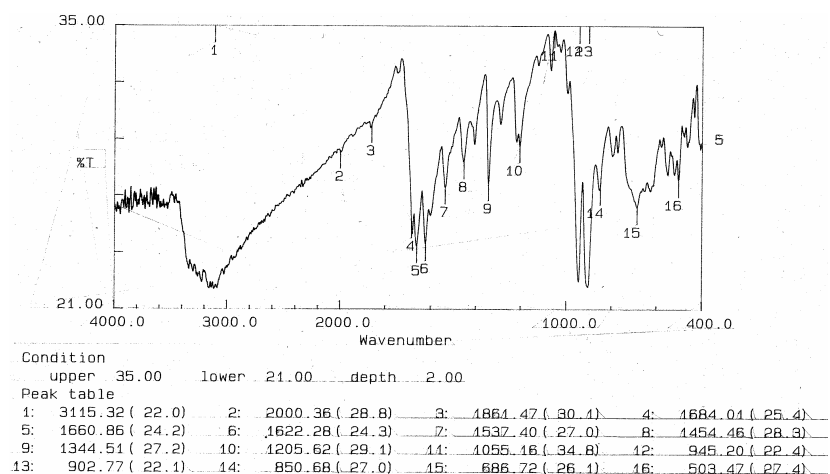


Figure S7. IR spectrum of compound 1

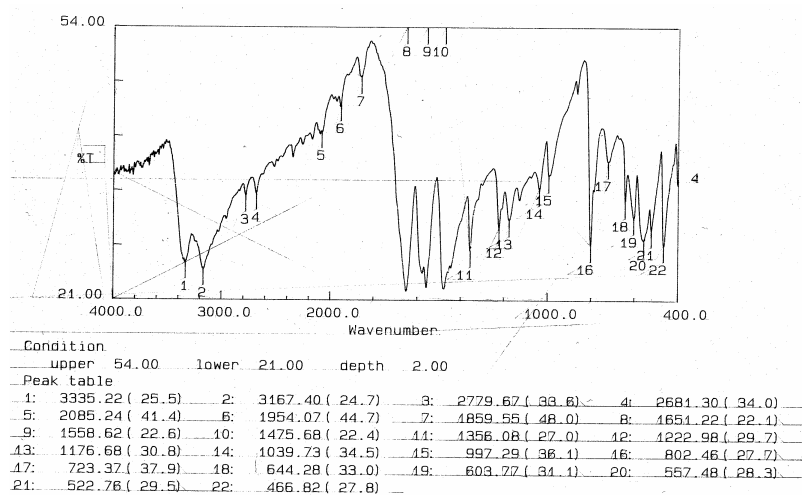


Figure S8. IR spectrum of 2-aminopyrimidine

*****End of Supplementary materials*****