Title:	Carbinol mediated clusterization of Nickel(II) ions in a Schiff base backbone: Structural & solution properties, phosphoester cleavage activity including theoretical support
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Abstract:	In this study, the significant role of carbinol in the construction of a tetranickel(II) cluster, [Ni4II(μ-OHCH3)2(L)2(CH3OH)2]·2CH3OH (1) with a compartmental Schiff base, [H3L = N,N′-bis(3-methoxysalicylidene)-1,3-diamino-2-propanol] is reported and emphasized. The tetranickel cluster crystallizes in a monoclinic system with P21/n space group. The tetranickel(II) core exists in a dicubane structure adopting octahedral geometry for each nickel(II) centres. In forming tetrametallic core, carbinol as solvent molecules exhibit its uniqueness through versatile coordination motifs (bridging-, terminal- and solvent of crystallization) in assembling four nickel(II) ion with two Schiff base units. Hirshfeld analysis for 1 defines pivotal role of MeOH in construction of long range crystalline architecture. Examination of its ability towards cleavage of phosphoesterase bonds using 4-nitrophenylphosphate (PNPP) in carbinol authenticates its excellent cleavage efficiency with rate constant 1.61 × 10−4 min−1. Presence of coordinated methanol molecules at Ni(II) centre as well as multiple reaction centres in tetra-nickel(II) core remain the driving force for the phosphatase activity. Outcomes from extensive density functional theory (DFT) justify well the experimental observations.
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