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**Title:** Synthesis and spectroscopic characterization of a photo-stable tetrazinc(II)â€ŠSchiff base cluster: A rare case of ligand centric phenoxazinone synthase activity

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**Abstract:** Herein, the synthesis, structural characterization and catalytic activity of a novel tetranuclear zinc(II)–Schiff base complex,  $[Zn_4(L)_2(\mu_3-OCH_3)_2(CH_3OH)_2] \cdot 2CH_3OH$  (1), [L = N,N'-bis(3-methoxysalicylidene)-1,3-diamino-2-propanol] was presented. Single crystal X-ray diffraction structural analysis revealed that the tetra-zinc(II) cluster crystallized in a monoclinic system with P21/c space group. Interestingly, three different molecular bridges (methoxido-, alkoxido- and phenoxido-) simultaneously co-existed in assembling tetra-zinc(II) core, which was a very rare observation. To the best of our knowledge, this compound would be the first compound where a diverse coordination aspect was covered by a single solvent as terminal coordinator (CH<sub>3</sub>OH), bridging ( $\mu_3$ -CH<sub>3</sub>OH) and solvent for crystallization in the existing scientific literature. The compound showed good photo-stability and excellent luminescence property with higher lifetime at transition state in ethanol. This zinc(II) complex revealed crucial role as an effective catalytic system towards oxidation of 2-aminophenol (2-AP) in ethanol. Additionally, the tetra-zinc(II) complex displayed potential phenoxazinone synthase like activity with momentous turn over number,  $k_{cat}$  ( $h^{-1}$ ) =  $6.19 \times 10^2$  in ethanol under aerobic condition. ESI-MS and EPR spectral analysis of the reaction mixture between Zn(II) complex and 2-AP recommended that the course of catalysis proceeded through substrate–catalyst adduct formation and authenticated the radical mechanistic pathway in favor of oxidative coupling product. This tetranuclear zinc(II)–Schiff base complex would be considered as the first example that catalyzed the oxidative coupling of 2-aminophenol to aminophenoxazino compound under usual aerobic condition. As complementary, detailed quantum chemical computations, performed with density functional theory (DFT) were well corroborated with the experimental results. This was the first and rarest example where a tetrazinc(II)–Schiff base cluster exhibited catalytic oxidation of 2-AP through ligand centered radical activity.

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