Title:	Transesterification activity by a zinc(II)-Schiff base complex with theoretical interpretation
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Abstract:	The article demonstrates the synthesis, structural characterization and transesterification activity of a mononuclear zinc(II) complex, [Zn(HL)(H2O)]·(H2O) (1) containing a previously reported Schiff base ligand, H3L = N,N′-bis(salicylidene)-1,3-diamino-2-propanol]. X-ray structural analysis of 1 reveals that Zn(II)-Schiff base complex crystallizes in hexagonal crystal system with P61 space group and adopts a distorted tetrapyramidal geometry. Self-assembled molecular units of 1 exhibit a beautiful construction of 3D crystalline architecture through intermolecular hydrogen bond wire. Zinc(II) complex displays an enhancement of fluorescence intensity in comparison to HL in methanol medium. Catalytic behaviour of 1 towards disodium salt of 2,4-dinitrophenylphosphate (PNPP) in aqueous-methanol medium exhibits good transesterification activity with initial rate constant value of 1.73 × 10−4 min−1. Detailed DFT calculations are also employed to cope with the geometrical parameters of 1 as well as to explore the proposed catalytic mechanism of transesterification activity.
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