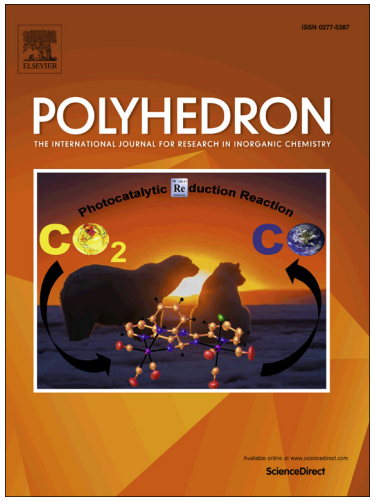

Modulation in π · · · π, cation· · · π and C–H· · ·H–C interactions varying the counter anions in square planar nickel(II) Schiff base complex: A combined experimental and theoretical study

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Modulation in π···π, cation···π and C–H···H–C interactions varying the counter anions in square planar nickel(II) Schiff base complex: A combined experimental and theoretical study

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Abstract: Two mononuclear square planar nickel(II) complexes, *[Ni(HL)$_2$](ClO$_4$)$_2$* (**1**) and *[Ni(HL)$_2$]Cl$_2$·2H$_2$O* (**2**), [where HL = 3-(dimethylaminopropyliminomethyl)naphthalen-2-ol] have been synthesised and characterized by elemental and spectral analysis. The structures have been confirmed by single-crystal X-ray diffraction. In each complex, the Schiff base is present in its zwitter ionic form. Interesting supra-molecular networks were generated through various non-covalent forces. Density functional theory (DFT) calculations were employed to estimate the contribution of each interaction in the formation of the assembly using several theoretical models.

Keywords: Nickel(II); Schiff base; Crystal structure; DET study; Non-covalent interactions.