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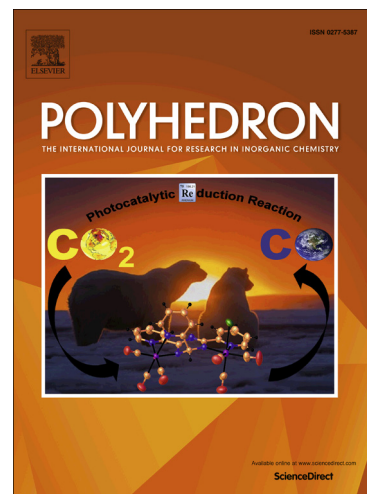
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Modulation in $\pi\cdots\pi$, cation $\cdots\pi$ and C–H $\cdots$ H–C interactions varying the counter anions in square planar nickel(II) Schiff base complex: A combined experimental and theoretical study

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Abstract: Two mononuclear square planar nickel(II) complexes, $[Ni(HL)_2](ClO_4)_2$ (**1**) and $[Ni(HL)_2]Cl_2 \cdot 2H_2O$ (**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.

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