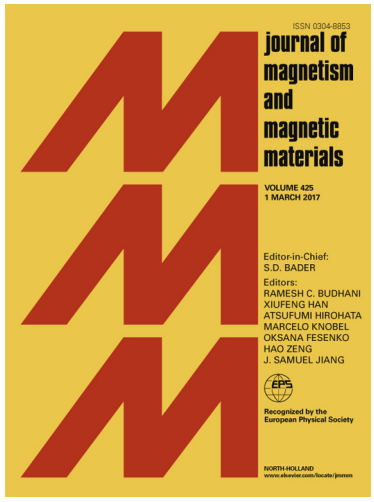

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Magnetic interaction in a 2D solid through hydrogen bonds and π-π stacking

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Abstract. The intercalation of pyridine and its 3-substituted halogen derivatives (L) between layers of nickel (T) tetracyanonickelate provides a beautiful example of magnetic interaction through π-π stacking. The intercalation process results in the formation of 3D solids with formula unit $TL_2[Ni(CN)_4]$. In the interlayer region, the intercalated molecules are found coordinated to the axial positions for the metal T (Ni). Neighboring molecules remain interacting through their dipole and quadrupole moments. For a coplanar configuration of their aromatic rings, the corresponding π-π clouds appear overlapped, which makes possible the appearance of a weak ferromagnetic interaction between T metal centers, to form an ordered system of magnetic chains separated about 10 Å. The halogen substituent in the pyridine molecule modulates the π-π clouds overlapping and, in consequence, the magnetic interaction through the chain. Such interaction coexists with a weak antiferromagnetic coupling between T atoms through the CN bridges in the two dimensional system, $\{T[Ni(CN)_4]\}_\infty$, but at low temperature, the interaction through the π-π clouds overlapping dominates. This contribution includes the study of the magnetic properties of the layered $T(H_2O)_2[Ni(CN)_4]\cdot xH_2O$ precursor solid where the magnetic interaction takes place through the hydrogen bonding network formed by the water molecules found in the interlayer region. The magnetic properties of both series of layered solids were evaluated from low temperature SQUID measurements complemented with structural and spectroscopic information. The interpretation of the magnetic and structural data is supported by computational calculations on the intermolecular interactions in the interlayer region.

Keywords: Molecular magnets; Intercalation compounds; hybrid inorganic-organic solids; pi-pi coupling.