Poster

Synthesis, crystal structure, Hirshfeld surface analysis and framework Energy study of a new Ni-Coordination complex with 1,10-phenanthroline

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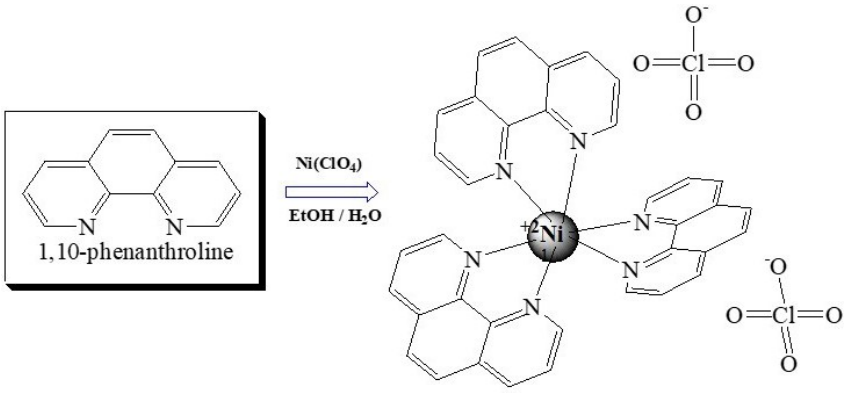
In recent years, there has been a significant surge in the exploration of metal complexes containing biologically active ligands, with a focus on both their biological applications and structural intricacies. Notably, complexes incorporating 1,10-phenanthroline show promise in combating cancer through DNA intercalation [1], while synthetic nickel (II) complexes are being investigated for their potential in medicinal applications, particularly in inhibiting cancer cell proliferation [2].

1,10-phenanthroline (phen) is a well-known bidentate ligand in coordination chemistry, prized for its tricyclic, aromatic, N-heterocyclic structure. This structure possesses unique attributes, including an electron-deficient heteroaromatic system and a rigid planar structure induced by the central ring, facilitating rapid complex formation with metal ions [3-4a,b].

In our study, we synthesized a novel coordination complex, $[Ni(Phen)_3](ClO_4)_2$, using nickel salt, sodium azide, and 1,10-phenanthroline in an ethanol-water mixture at room temperature (scheme-1). Structural analysis reveals that:

The compound crystallizes in the triclinic space group P-1, with Ni(II) ions coordinated by six N-donor atoms from three 1,10-phenanthroline ligands, balanced by the inclusion of two perchlorate anions.

The resulting complex underwent characterization via single-crystal X-ray diffraction, revealing rich intermolecular interactions driven by the aromatic ring in phenanthroline and the hydrogen bond acceptor effect induced by perchlorate anions. The network is elucidated using Hirschfeld Surface analysis and Energy of framework calculation, highlighting the predominant involvement of O… H/O..H contacts in the crystal structure networks. Confirming the role of these interactions in the cohesion of the crystalline structure.



Scheme 1. Synthesis and coordination mode of the complexes $[Ni(Phen)_3](ClO_4)_2$.

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