Poster

Structural Design, Hirshfeld Analysis And Noncovalent Interactions of Newly Synthesized Ni(II) Complex With A Dithiocarbazate Ligand

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The present work reports the synthesis and structural design of a new Ni(II) complex [Ni(L)PPh_3] with the S-benzyl-2-(2-hydroxyphenyl-ethylidene)dithiocarbazato (H_2L) ligand. The metal complex was characterized by single-crystal X-ray diffraction, FT- IR, UV-Vis, and ^{1}H nuclear magnetic resonance. Single crystal X-ray analysis revealed a mononuclear complex with distorted square planar geometry and the metal center coordinated with a doubly deprotonated dithiocarbazate molecule and a coligand triphenylphosphine molecule [1-3]. The Schiff base is coordinated by the *ONS*-donor system to the metal center. The noncovalent interactions were investigated by the Hirshfeld surface and revealed intermolecular hydrogen bonds and $\pi\cdots\pi$ stacking interactions (Figure 1). Anticancer activity of the free ligand and its Ni(II) complex was evaluated on human breast cancer cell line MCF-7 and non-malignant breast epithelial cell line MCF-10A. The complex demonstrated lower IC_{50} values for malignant breast cell lines than their non-malignant counterparts with strong potency in inhibiting cancerous cells.

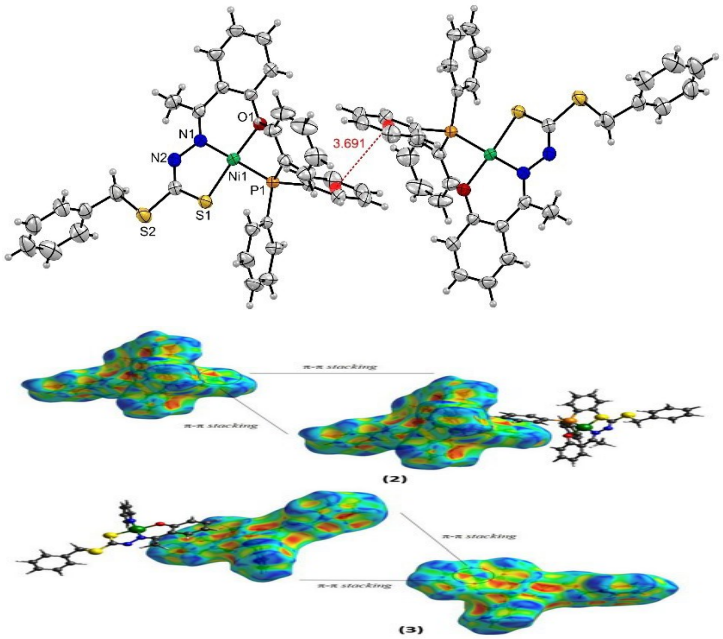

Figure 1. Projection view of the complex [Ni(L)PPh_3] showing the $\pi\cdots\pi$ stacking interactions and Hirshfeld surface mapped in shape index.

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[2] Cavalcante, C. D. Q. O.; Garcia, E.; da Mota, T. H. A.; de Oliveira, D. M.; Gatto, C. C.; *J. Inorg. Biochem.* **2022**, *237*, 112015.

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