MS14-P17 | Preparation, Spectral, Structural, Hirshfeld surface and molecular docking of tetrakis(pyridine-κN)bis(thiocyanato-κN) cobalt(II) complex

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The structure of the title complex, $[Co(NCS)_2(C_5H_5N)_4]$ was synthesized, studied by FTIR, UV-visible and single crystal X-ray diffraction analysisre. The asymmetric unit of compound, consists of one cobalt(II) cation, one thiocyanate anions and two pyridine ligands. In the structure of cobalt complex, the cobalt(II) cations are octahedrally coordinated by two terminal N-bonding thiocyanate anions and by the N atoms of four pyridine ligands, resulting in discrete and slightly distorted octahedral complex. The complexes are linked into a three-dimensional network via intremolecular hydrogen bonds Interactions C-H···S, C-H···C, and π-π stacking interactions [centroid–centroid distances = 3.753 A°] between pyridine ring systems. The diferent intermolecular interactions studied through Hirshfeld surface analysis enables contributions to the crystal packing of the cobalt complex to be quantified. The shemes 2D and 3D, associated with the Hirshfeld surface clearly display each significant interaction involved in the structure, by quantifying them in an effective visual manner. The molecular docking studies were also performed against various cancer target proteins 4FLH (colon cancer), 1SVC (pancreatic cancer), 1MOX (lung cancer) and 2DSQ (breast epithelian cancer). The complex showed good molecular interactions with all the receptors.