# SYNTHESIS, CRYSTAL STRUCTURE, AND HIRSHFELD SURFACE ANALYSIS OF A BIS (1,10-PHENANTHROLINE) MANGANESE(II) COMPLEX

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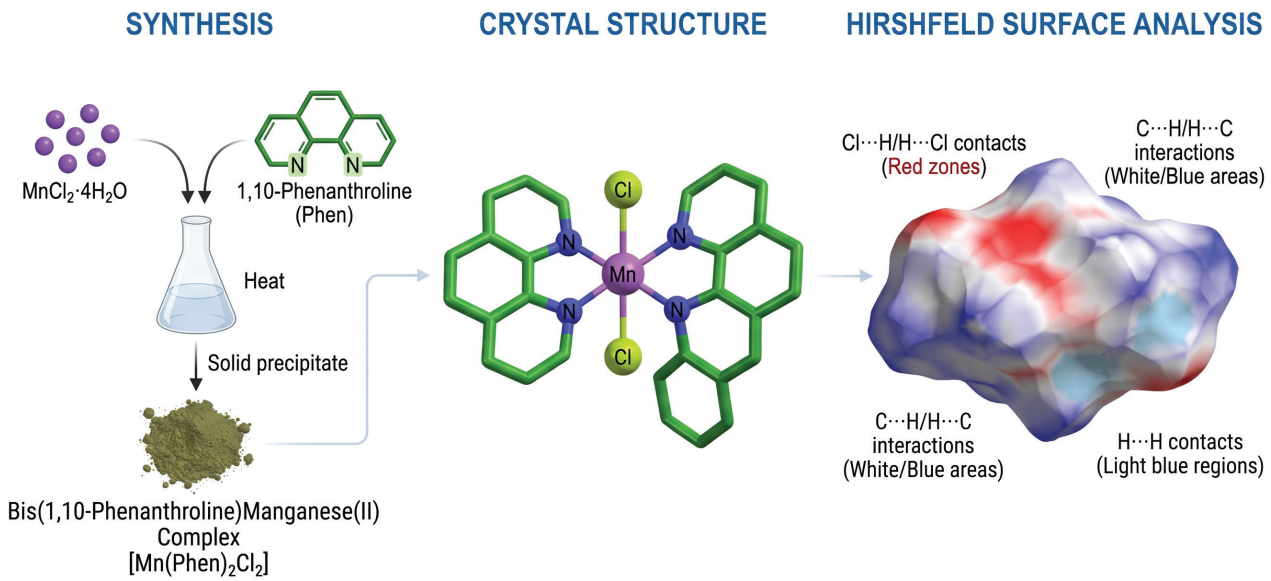
TerSU



## Annotation.

***The bis(1,10-phenanthroline) manganese(II) complex, [Mn(Phen)2Cl2], was successfully synthesised and comprehensively characterised by single-crystal X-ray diffraction, powder X-ray diffraction (PXRD), and Hirshfeld surface analysis. Single-crystal X-ray diffraction revealed that the complex crystallises in the monoclinic crystal system, with the Mn(II) centre adopting a distorted octahedral coordination geometry formed by four nitrogen atoms from two bidentate 1,10-phenanthroline ligands and two chloride ions. PXRD analysis confirmed the phase purity of the synthesised compound and demonstrated excellent agreement between the experimental and simulated diffraction patterns, indicating a highly ordered crystalline structure. Hirshfeld surface analysis indicated that the crystal packing is mainly governed by H···H, C···H/H···C, and Cl···H/H···Cl intermolecular contacts, highlighting the important role of van der Waals and electrostatic interactions in stabilising the crystal structure. The combined structural analyses provide a comprehensive understanding of the molecular geometry, intermolecular interactions, and crystal packing of the title manganese(II) complex.***



## Key words:

***CCD Xcalibur Ruby, Hirshfeld surface analysis, XRD, 1,10-phenanthroline***


## Introduction.

In recent years, there has been a sharp increase in scientific interest in metal-organic complexes (MOCs)[1] due to limitations such as the insufficient efficiency and selectivity of materials widely used in fields such as catalysis, gas separation, and storage, and their low thermal and chemical stability. Complex compounds based on metal-ligand coordination form a wide class of compounds with various chemical structures and properties, including MOCs - complex compounds formed as a result of coordination bonds between central metal ions and multi-toothed (dentate) organic ligands, which belong to the class of discrete coordination clusters with a specific geometric structure, specific porous cavities, nanoscale structures, and symmetrical geometry (e.g., octahedral, tetrahedral, or cuboqtahedral)[2]. The metal-ligand coordination bond allows for the production of high-quality and defect-free products under environmental conditions compared to synthesis strategies based on classical covalent bonds. The work of Fujita , Stang, Newkome, Nitschke, and other researchers formed the fundamental basis for the synthesis of metal-organic complexes, which developed new coordination compounds, including three-dimensional metal-organic cage (MOC) structures with different geometries, such as a triangle, a rectangle[3], a square, a rhomboid, a cube, an octahedron, a cuboctahedron, a trigonal prism, a tetragonal prism, and a hexagonal prism[4].

The bis(1,10-phenanthroline)manganese(II) complex, $[Mn(Phen)_2Cl_2]$, synthesised using the bidentate 1,10-phenanthroline ligand, was identified as a new coordination compound and structurally characterised by single-crystal X-ray diffraction analysis[5]. The crystallographic study revealed that the Mn(II) centre adopts a distorted octahedral coordination geometry formed by four nitrogen atoms from two 1,10-phenanthroline ligands and two chloride ions. In addition, the crystal structure analysis provided valuable information on the supramolecular architecture, showing that

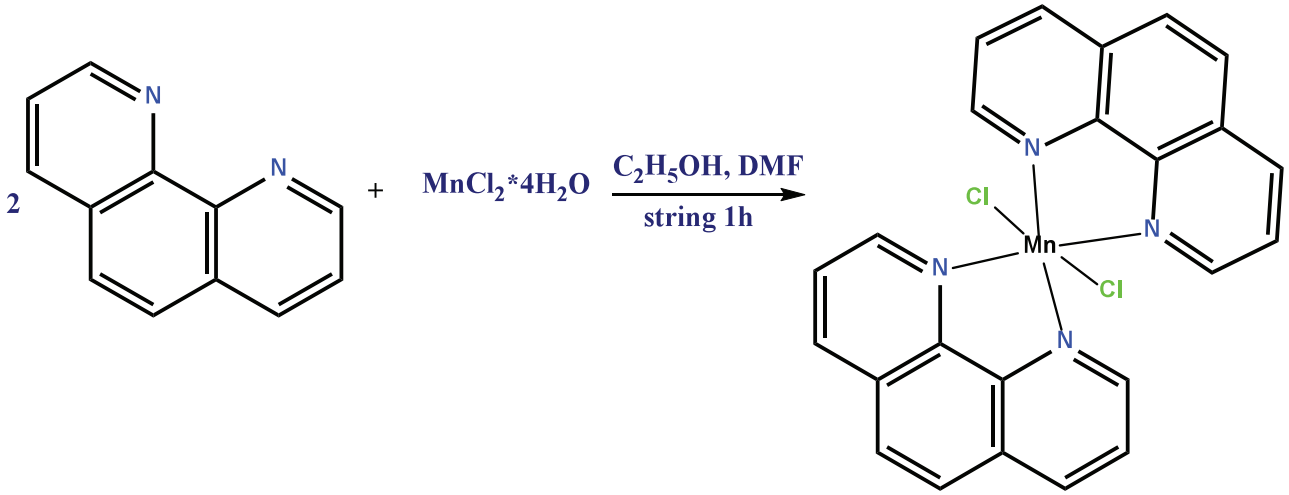
1 D.K. Saidov, K.K. Turaev, S.A. Kasimov, A. Kumar, B.Z. Adizov, Y.Y., Yakubov, B.T., Ibragimov, A., Lakshmanan, A.S., Normamatov, B.D. Mamatkodirov, J. Gao, Cd(II)-based 2D coordination polymer with hydroxynaphthoate: Synthesis, DFT insights, and surface analysis, J. Mol. Struct. (2025) 145225. https://doi.org/10.1016/j.molstruc.2025.145225.

2 D.Kh. Saidov, Kh.Kh. Turaev, A.B. Ibragimov, G.Kh. Toirova, Kh. Kh. Kulbasheva, Synthesis, thermal, Hirshfeld surface analysis, and spectroscopic properties of a Cd(II) coordination polymer with 1-hydroxy-2-naphthoic acid, Int. J. Eng. Trends Technol. 73(7) (2025) 293-307, https://doi.org/10.14445/22315381/IJETT-V73I7P123.

3 Ugli Saidov, DK, Turaev, KK, Kumar, A., Kasimov, S.A., Adizov, B.Z., Yakubov, Y.Y., ... & Ibragimov, A.B. (2026). Synthesis, Structural Characterization, and Antimicrobial Activity of Cadmium (II) Coordination Polymer Derived from 1, 10-Phenanthroline and Tartaric Acid. Journal of Molecular Structure, 146200. https://doi.org/10.1016/j.molstruc.2026.146200

4 ugli Saidov, DK, Turaev, KK, Kumar, A., Kenjayevna, SZ, Ugli Kholturaev, KB, Ugli Ruziev, UU, ... & Chellakarungu, B. (2026). Structural elucidation, supramolecular interactions, and antifungal activity of a one-dimensional Cu (II) coordination polymer based on 1, 10-phenanthroline and isonicotinate. Journal of Solid State Chemistry, 126074. https://doi.org/10.1016/j.jssc.2026.126074

5 A.R. Safarov, H. Ferjani, YG.Abou El-Reash, A.B. Ibragimov, Y.R. Takhirov, Kh.Kh. Turaev, D Kh. Saidov, T.A. Yousef, B.Z. Adizov ,Ch. Balakrishnan. Structural, spectroscopic, and Hirshfeld surface analysis of novel zinc(II) complexes with aminobenzoate and thiadiazole units. Polyhedron 15 February 2026 https://doi.org/10.1016/j.poly.2026.118038




the crystal packing is stabilised by intermolecular C–H···Cl interactions, weak π···π stacking between neighbouring phenanthroline rings, and van der Waals forces. These structural features play an important role in determining the stability and physicochemical properties of the complex[1].

## Experimental.

A total of 0.1802 g (0.05 mmol) of 1,10-phenanthroline was completely dissolved in a mixed solvent of 20 mL 96% ethanol and 10 mL dimethylformamide (DMF). Separately, 0.297 g (0.05 mmol) of manganese(II) chloride tetrahydrate ($MnCl_2•4H_2O$) was dissolved in 30 mL of distilled water, and the resulting solution was slowly added dropwise to the ligand solution under continuous stirring. The reaction mixture was stirred for 1 hour using a magnetic stirrer to ensure complete complexation. Subsequently, the mixture was subjected to ultrasonic treatment for 45 minutes employing an ultrasonic cleaner operating at 100 W power and 40 kHz frequency, which facilitated homogenisation and sterilisation of the solution. The resulting solution was then filtered through filter paper to obtain a clear, colourless filtrate. For crystallisation, the filtrate was stored in a thermostat at 40-50 °C for 25 days, allowing slow evaporation of the solvents and promoting the growth of well-defined crystals. As a result, light pink, sharply faceted crystals were obtained with a total yield of 76% (Scheme 1).

## Results and discussion.

Single-crystal XRD analysis. Crystal Structure Description:

The experimental conditions for single-crystal X-ray diffraction and subsequent structure refinement are presented in Table 1, while Table 4 lists the key bond lengths and bond angles. The $[Mn(Phen)_2Cl_2]$ complex crystallizes in the triclinic crystal system with a noncentrosymmetric space group P1, reflecting a low-symmetry crystal environment and a slightly distorted molecular geometry within the lattice. The molecular structure of the $[Mn(Phen)_2Cl_2]$ complex is shown in figure 1(a), with displacement ellipsoids drawn at the 50% probability level, and atoms labelled according to the standard numbering scheme.

Single-crystal X-ray diffraction analysis reveals that the $[Mn(Phen)_2Cl_2]$ complex is a mononuclear molecular compound. In this structure, the $Mn^{2+}$ ion adopts a distorted octahedral geometry, being coordinated by four nitrogen atoms from two bidentate 1,10-phenanthroline (Phen) ligands and two chloride ions.

Each Phen ligand chelates the $Mn^{2+}$ center through its two nitrogen atoms ($\kappa^2N,N`$), while the chloride ions occupy the remaining coordination sites, completing the octahedral environment. This bidentate and monoatomic coordination results in a slightly distorted molecular geometry rather than an extended polymeric network.

The Mn-N bond lengths range from 2.252(3) to 2.396(3) Å, while the Mn-Cl distances are slightly longer, 2.4176(15)-2.4857(10) Å, reflecting the weaker ionic character of the Mn-Cl bonds compared to Mn-N chelation. The average bond length of 2.3586 Å is consistent with typical six-coordinate Mn(II) complexes. The polyhedral volume of the Mn coordination sphere is 16.4987 $Å^3$, indicating a moderately compact environment. The distortion index (0.03164) and quadratic elongation (1.0411) quantitatively confirm a slight distortion from ideal octahedral geometry, which is further supported by the bond angle variance of 131.21 °[2]. The effective coordination number of 5.6742 reflects that while Mn is nominally six-coordinate, small deviations in bond lengths reduce the "effective" coordination slightly below six (Table 3, figure. (1b).

1 ugli Juraev, AS, Khamidjanovich, RA, Prasad, AA, Turaev, KK, ugli Ruziev, UU, ugli Kholturaev, KB, ... & Balakrishnan, C. (2026). Synthesis, crystal structure, supramolecular architecture, and electronic structure analysis of a new iron (III)-EDTA complex salt. Journal of Molecular Structure, 146273. https://doi.org/10.1016/j.molstruc.2026.146273

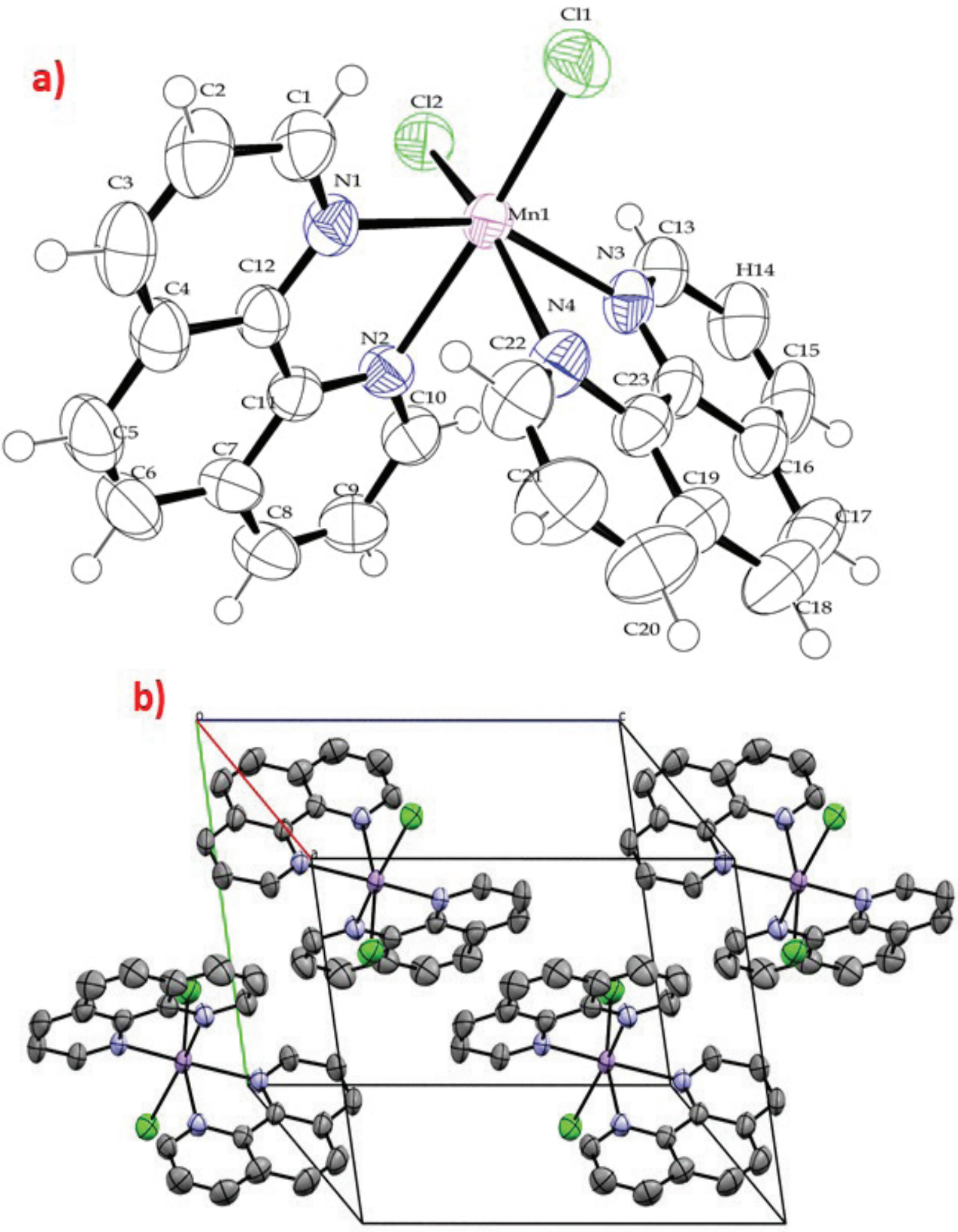



**Fig. 1**

**(a) ORTEP of the asymmetric unit of [Mn(Phen)2Cl2], showing the atom-numbering scheme with displacement ellipsoids drawn at the 50% probability level.**

**(b) Crystal packing diagram.**

Table 1.

## Crystal data and structure refinement details for $[Mn(Phen)_2Cl_2]$

| Crystal Data | |
|---|---|
| Formula | $C_{24}H_{16}Cl_2MnN_4$ |
| Formula Weight | 194.50 |
| Crystal System | triclinic |
| Space group | P-1 (No.2) |
| a, b, c [Å] | 9.2112(8), 0.0258(8), 12.6224(9) |
| α, β, γ (°) | 79.907(6), 81.073(6), 69.933(7) |
| V [Å$^3$] | 1072.26(16) |
| Z | 5 |
| D (calc) [g/cm$^3$] | 1.506 |
| Mu [mm$^{-1}$] | 7.450 |
| F(000) | 494 |
| Crystal Size [mm] | 0.05 x 0.20 x 0.30 |
| **Data Collection** | |
| Temperature (K) | 293 |
| Radiation [Å] | CuKα 1.54184 |
| Theta Min-Max [°] | 3.6, 67.7 |
| Dataset | -10: 11 ; -11: 12 ; -15: 14 |
| Tot., Uniq. Data, $R_{(int)}$ | 6658, 3814, 0.031 |
| Observed Data [I > 0.0 sigma(I)] | 3276 |
| **Refinement** | |
| $N_{ref}$, $N_{par}$ | 3814, 280 |
| R, wR2, S | 0.0570, 0.1645, 1.04 |
| Max. and Av. Shift/Error | 0.00, 0.00 |
| Min. and Max. Resd. Dens. [e/Ang$^3$] | -0.29, 0.88 |
| **CCDC** | **2497019** |

**Table 2 - Hydrogen Bonds (Angstrom, Deg)**

| D-H•••A | d(D-H) | d(H•••A) | d(D•••A) | <(DHA) |
|---|---|---|---|---|
| C(8)-H(8)•••Cl(2) | 0.9300 | 2.6900 | 3.610(5) | 170.00 |
| C(20)-H(20)•••Cl(2) | 0.9300 | 2.8000 | 3.696(6) | 161.00 |

Table 3.

*Polyhedral parameters for [Mn(Phen)$_2$Cl$_2$]*

| Bond distance (Å) | |
|---|---|
| Mn(1)-N(3) | 2.252(3) |
| Mn(1)-N(1) | 2.258(4) |
| Mn(1)-N(2) | 2.342(4) |
| Mn(1)-N(4) | 2.396(3) |
| Mn(1)-Cl(1) | 2.4176(15) |
| Mn(1)-Cl(2) | 2.4857(10) |
| Average bond length (Å) | 2.3586 |
| Polyhedral volume Å^3 | 16.4987 |
| Distortion index (bond length) | 0.03164 |
| Quadratic elongation | 1.0411 |
| Bond angle variance deg.^2 | 131.2122 |
| Effective coordination number | 5.6742 |

Table 4.

*Theselectedbondlengths(Å),angles(°)anddihedralangles(°)for [Mn(Phen)$_2$Cl$_2$]*

| Bond | Length[Å] | Bond | Length[Å] |
|---|---|---|---|
| Mn1-Cl1 | 2.4176(14) | C5-C6 | 1.355(7) |
| Mn1-Cl2 | 2.4857(11) | C6-C7 | 1.441(7) |
| Mn1-N1 | 2.258(3) | C7-C8 | 1.413(7) |
| Mn1-N2 | 2.342(3) | C7-C11 | 1.394(6) |
| Mn1-N3 | 2.252(3) | C8-C9 | 1.352(7) |
| Mn1-N4 | 2.396(3) | C9-C10 | 1.393(7) |
| N1-C1 | 1.323(5) | C11-C12 | 1.442(5) |
| N1-C12 | 1.360(5) | C13-C14 | 1.399(6) |
| N2-C10 | 1.324(5) | C14-C15 | 1.353(9) |
| N2-C11 | 1.363(5) | C15-C16 | 1.405(7) |
| N3-C13 | 1.328(5) | C16-C17 | 1.438(8) |
| N3-C24 | 1.352(5) | C16-C24 | 1.419(5) |
| N4-C22 | 1.338(5) | C17-C18 | 1.344(8) |
| N4-C23 | 1.363(5) | C18-C19 | 1.438(7) |
| C1-C2 | 1.399(6) | C19-C20 | 1.410(8) |
| C2-C3 | 1.358(8) | C19-C23 | 1.397(7) |
| C3-C4 | 1.411(6) | C20-C21 | 1.377(8) |
| C4-C5 | 1.424(8) | C21-C22 | 1.382(8) |
| C4-C12 | 1.406(6) | C23-C24 | 1.449(6) |

Symmetry transformations used to generate equivalent atoms: a = 1-x, 1-y,1-z, b = 1+x,y,z, c = 1+x,-1+y,z, d = 1-x,-y,-z, e = 1-x,-y,1-z, f = 1-x,1-y,-z, g = x,y,-1+z, h = -x,1-y,-z, i = -1+x,y,z, j = -x,-y,1-z, k = -x,1-y,1-z, l = x,y,1+z, m = -x,-y,-z, n = -1+x,1+y,z

| Bond | Angle[°] | Bond | Angle[°] |
|---|---|---|---|
| Cl1-Mn1-Cl2 | 103.27(4) | C1-C2-C3 | 119.3(4) |
| Cl1-Mn1-N1 | 95.51(9) | C2-C3-C4 | 119.6(4) |
| Cl1-Mn1-N2 | 165.85(7) | C3-C4-C5 | 123.4(4) |
| Cl1-Mn1-N3 | 101.61(10) | C3-C4-C12 | 117.3(4) |
| Cl1-Mn1-N4 | 94.85(9) | C5-C4-C12 | 119.3(4) |
| Cl2-Mn1-N1 | 103.12(8) | C4-C5-C6 | 121.1(5) |
| Cl2-Mn1-N2 | 86.34(8) | C5-C6-C7 | 120.9(5) |
| Cl2-Mn1-N3 | 95.34(8) | C6-C7-C8 | 123.6(5) |
| Cl2-Mn1-N4 | 159.41(8) | C6-C7-C11 | 119.3(4) |
| N1-Mn1-N2 | 71.93(11) | C8-C7-C11 | 117.1(4) |
| N1-Mn1-N3 | 151.19(13) | C7-C8-C9 | 119.2(5) |
| N1-Mn1-N4 | 84.53(11) | C8-C9-C10 | 120.5(4) |
| N2-Mn1-N3 | 87.61(11) | N2-C10-C9 | 122.0(4) |
| N2-Mn1-N4 | 77.82(11) | N2-C11-C7 | 122.9(4) |
| N3-Mn1-N4 | 71.18(10) | N2-C11-C12 | 117.5(3) |
| Mn1-N1-C1 | 123.9(3) | C7-C11-C12 | 119.6(4) |
| Mn1-N1-C12 | 117.7(2) | N1-C12-C4 | 122.5(3) |
| C1-N1-C12 | 118.2(3) | N1-C12-C11 | 117.7(3) |
| Mn1-N2-C10 | 126.8(3) | C4-C12-C11 | 119.8(4) |
| Mn1-N2-C11 | 114.8(2) | N3-C13-C14 | 122.7(5) |
| C10-N2-C11 | 118.3(3) | C13-C14-C15 | 119.7(5) |
| Mn1-N3-C13 | 122.8(3) | C14-C15-C16 | 119.9(4) |
| Mn1-N3-C24 | 119.0(2) | C15-C16-C17 | 124.2(4) |
| C13-N3-C24 | 118.2(3) | C15-C16-C24 | 116.9(4) |
| Mn1-N4-C22 | 127.8(3) | C17-C16-C24 | 118.9(4) |
| Mn1-N4-C23 | 114.3(2) | C16-C17-C18 | 121.3(5) |
| C22-N4-C23 | 117.5(4) | C17-C18-C19 | 121.5(5) |
| N1-C1-C2 | 123.0(4) | C18-C19-C20 | 123.2(5) |
| C18-C19-C23 | 119.0(5) | N4-C23-C24 | 116.9(4) |
| C20-C19-C23 | 117.8(5) | C19-C23-C24 | 120.2(4) |
| C19-C20-C21 | 118.9(5) | N3-C24-C16 | 122.6(4) |
| C20-C21-C22 | 119.5(5) | N3-C24-C23 | 118.3(3) |
| N4-C22-C21 | 123.3(4) | C16-C24-C23 | 119.1(4) |
| N4-C23-C19 | 122.9(4) | | |

Symmetry transformations used to generate equivalent atoms: a = 1-x, 1-y,1-z, b = 1+x,y,z, c = 1+x,-1+y,z, d = 1-x,-y,-z, e = 1-x,-y,1-z, f = 1-x,1-y,-z, g = x,y,-1+z, h = -x,1-y,-z, i = -1+x,y,z, j = -x,-y,1-z, k = -x,1-y,1-z, l = x,y,1+z, m = -x,-y,-z, n = -1+x,1+y,z

| Dihedral bond | Angle [°] | Dihedral bond | Angle [°] |
|---|---|---|---|
| Cl1-Mn1-N1-C1 | 6.4(3)Cl1 | -Mn1-N1-C12 | -167.9(3) |
| Cl2-Mn1-N1-C1 | -98.6(3) | Cl2-Mn1-N1-C12 | 87.1(3) |
| N2-Mn1-N1-C1 | 179.7(3) | N2-Mn1-N1-C12 | 5.5(3) |
| N3-Mn1-N1-C1 | 132.9(3) | N3-Mn1-N1-C12 | -41.4(4) |
| N4-Mn1-N1-C1 | 100.8(3) | N4-Mn1-N1-C12 | -73.5(3) |
| Cl2-Mn1-N2-C10 | 73.5(3) | Cl2-Mn1-N2-C11 | -110.7(2) |
| N1-Mn1-N2-C10 | 178.5(3) | N1-Mn1-N2-C11 | -5.7(2) |
| N3-Mn1-N2-C10 | -22.1(3) | N3-Mn1-N2-C11 | 153.7(3) |
| N4-Mn1-N2-C10 | -93.3(3) | N4-Mn1-N2-C11 | 82.5(2) |
| Cl1-Mn1-N3-C13 | -86.6(4) | Cl1-Mn1-N3-C24 | 95.4(3) |
| Cl2-Mn1-N3-C13 | 18.1(4) | Cl2-Mn1-N3-C24 | -159.9(3) |
| N1-Mn1-N3-C13 | 148.1(4) | N1-Mn1-N3-C24 | -29.8(4) |
| N2-Mn1-N3-C13 | 104.2(4) | N2-Mn1-N3-C24 | -73.8(3) |
| N4-Mn1-N3-C13 | -177.9(4) | N4-Mn1-N3-C24 | 4.2(3) |
| Cl1-Mn1-N4-C22 | 81.3(4) | Cl1-Mn1-N4-C23 | -105.7(3) |
| Cl2-Mn1-N4-C22 | -126.9(3) | Cl2-Mn1-N4-C23 | 46.1(4) |
| N1-Mn1-N4-C22 | -13.8(4) | N1-Mn1-N4-C23 | 159.3(3) |
| N2-Mn1-N4-C22 | -86.4(4) | N2-Mn1-N4-C23 | 86.6(3) |
| N3-Mn1-N4-C22 | -178.0(4) | N3-Mn1-N4-C23 | -5.0(3) |
| Mn1-N1-C1-C2 | -174.4(3) | C12-N1-C1-C2 | -0.2(6) |
| Mn1-N1-C12-C4 | 175.0(3) | Mn1-N1-C12-C11 | -4.7(4) |
| C1-N1-C12-C4 | 0.5(6) | C1-N1-C12-C11 | -179.3(3) |
| Mn1-N2-C10-C9 | 173.5(3) | C11-N2-C10-C9 | -2.2(6) |
| Mn1-N2-C11-C7 | -173.9(3) | Mn1-N2-C11-C12 | 5.4(4) |
| C10-N2-C11-C7 | 2.3(6) | C10-N2-C11-C12 | -178.4(3) |
| Mn1-N3-C13-C14 | -177.4(4) | C24-N3-C13-C14 | 0.6(7) |
| Mn1-N3-C24-C16 | 177.3(4) | Mn1-N3-C24-C23 | -3.0(5) |
| C13-N3-C24-C16 | -0.7(7) | C13-N3-C24-C23 | 179.0(4) |
| Mn1-N4-C22-C21 | 173.2(4) | C23-N4-C22-C21 | 0.4(7) |
| Mn1-N4-C23-C19 | -175.3(4) | Mn1-N4-C23-C24 | 5.4(5) |
| C22-N4-C23-C19 | -1.5(7) | C22-N4-C23-C24 | 179.2(4) |
| N1-C1-C2-C3 | -1.2(7) | C1-C2-C3-C4 | 2.3(7) |
| C2-C3-C4-C5 | 179.1(5) | C2-C3-C4-C12 | -2.0(7) |
| C3-C4-C5-C6 | -178.5(5) | C12-C4-C5-C6 | 2.5(7) |
| C3-C4-C12-N1 | 0.6(6) | C3-C4-C12-C11 | -179.7(4) |
| C5-C4-C12-N1 | 179.6(4) | C5-C4-C12-C11 | -0.7(6) |
| C4-C5-C6-C7 | -2.6(7) | C5-C6-C7-C8 | -177.8(5) |
| C5-C6-C7-C11 | 0.7(7) | C6-C7-C8-C9 | 178.1(5) |
| C11-C7-C8-C9 | -0.4(7) | C6-C7-C11-N2 | -179.6(4) |
| C6-C7-C11-C12 | 1.1(6) | C8-C7-C11-N2 | -1.0(6) |
| C8-C7-C11-C12 | 179.7(4) | C7-C8-C9-C10 | 0.5(7) |
| C8-C9-C10-N2 | 0.8(7) | N2-C11-C12-N1 | -0.7(5) |
| N2-C11-C12-C4 | 179.6(4) | C7-C11-C12-N1 | 178.6(4) |
| C7-C11-C12-C4 | -1.1(6) | N3-C13-C14-C15 | -0.8(9) |

| | | | |
|---|---|---|---|
| C13-C14-C15-C16 | 1.1(9) | C14-C15-C16-C17 | 179.8(6) |
| C14-C15-C16-C24 | -1.3(8) | C15-C16-C17-C18 | -179.9(6) |
| C24-C16-C17-C18 | 1.1(9) | C15-C16-C24-N3 | 1.1(7) |
| C15-C16-C24-C23 | -178.6(5) | C17-C16-C24-N3 | -179.9(5) |
| C17-C16-C24-C23 | 0.4(7) | C16-C17-C18-C19 | -1.5(10) |
| C17-C18-C19-C20 | -179.6(6) | C17-C18-C19-C23 | 0.3(9) |
| C18-C19-C20-C21 | 178.9(6) | C23-C19-C20-C21 | -1.0(8) |
| C18-C19-C23-N4 | -178.1(5) | C18-C19-C23-C24 | 1.2(7) |
| C20-C19-C23-N4 | 1.8(8) | C20-C19-C23-C24 | -178.9(5) |
| C19-C20-C21-C22 | 0.0(9) | C20-C21-C22-N4 | 0.3(9) |
| N4-C23-C24-N3 | -2.0(6) | N4-C23-C24-C16 | 177.8(4) |
| C19-C23-C24-N3 | 178.7(4) | C19-C23-C24-C16 | -1.6(7) |

Symmetry transformations used to generate equivalent atoms: a = 1-x, 1-y,1-z, b = 1+x,y,z, c = 1+x,-1+y,z, d = 1-x,-y,-z, e = 1-x,-y,1-z, f = 1-x,1-y,-z, g = x,y,-1+z, h = -x,1-y,-z, i = -1+x,y,z, j = -x,-y,1-z, k = -x,1-y,1-z, l = x,y,1+z, m = -x,-y,-z, n = -1+x,1+y,

***Powder XRD analysis***To assess the degree of crystallinity and phase purity of the [Mn(phen)$_2$Cl$_2$] complex, X-ray diffractometry (PXRD) analysis in powder form was conducted (See Figure 2). The measured experimental diffractogram data were compared with the modelled diffractogram based on X-ray diffraction data obtained for a single crystal. The results show that there is a high degree of correspondence between the two diffractograms in terms of the location of the main peaks at the 2θ angles. This fact scientifically confirms that the crystalline structure of the synthesised powder sample fully corresponds to the phase in a single crystalline state. The directional growth of crystalline particles or differences in their size and morphological properties explain small differences in peak intensities. In general, the high degree of correspondence between the experimental and simulated diffractograms reliably confirms the phase purity and crystal structure stability of the [Mn(phen)$_2$Cl$_2$] complex.

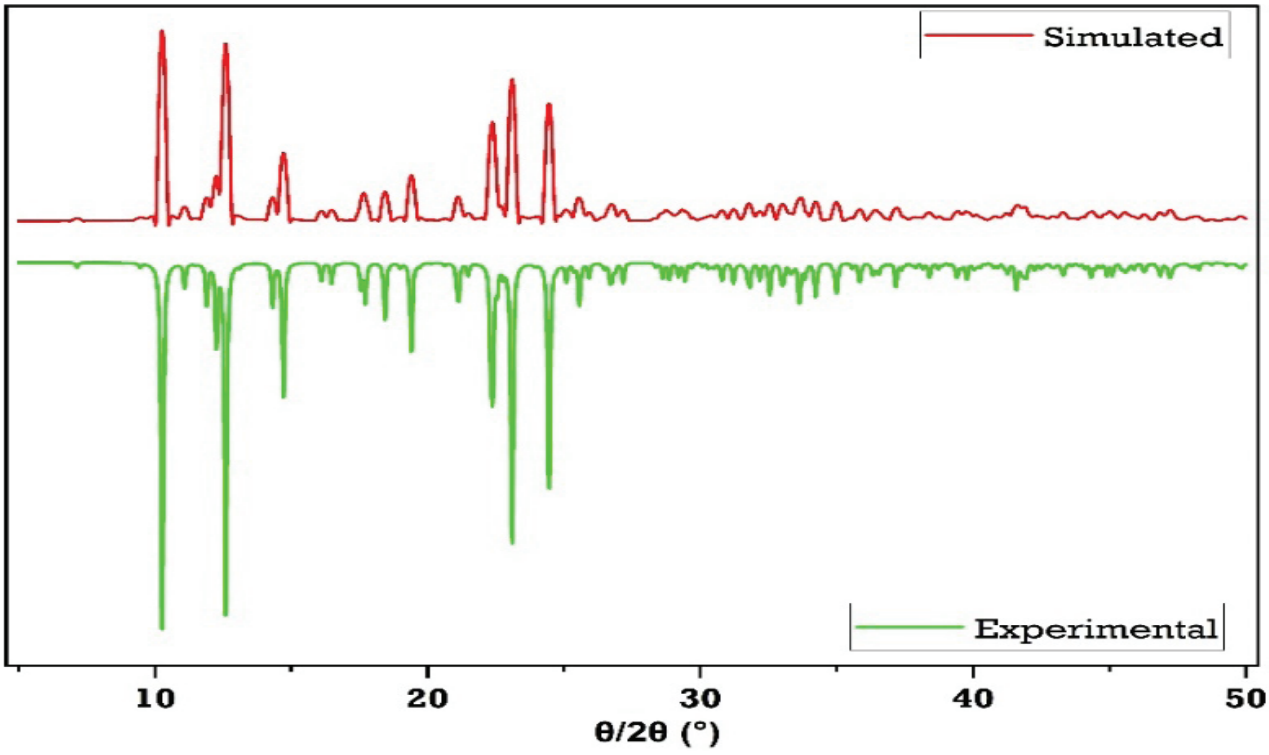



**Fig.2**

***Simulated PXRD patterns and experimental XRD patterns of the [Mn(phen)$_2$Cl$_2$]***

## Hirshfeld surface analysis

Hirshfeld surface analysis was carried out to determine the nature of intermolecular interactions within the crystal structure and to assess their contribution to overall stability. This method allows you to identify the most important contacts by analyzing the distribution of electron density around the molecule. The results are presented in Hirshfeld surface maps (See Figure 3) and fingerprint graphs (See Figure 4) were analyzed visually and quantitatively.

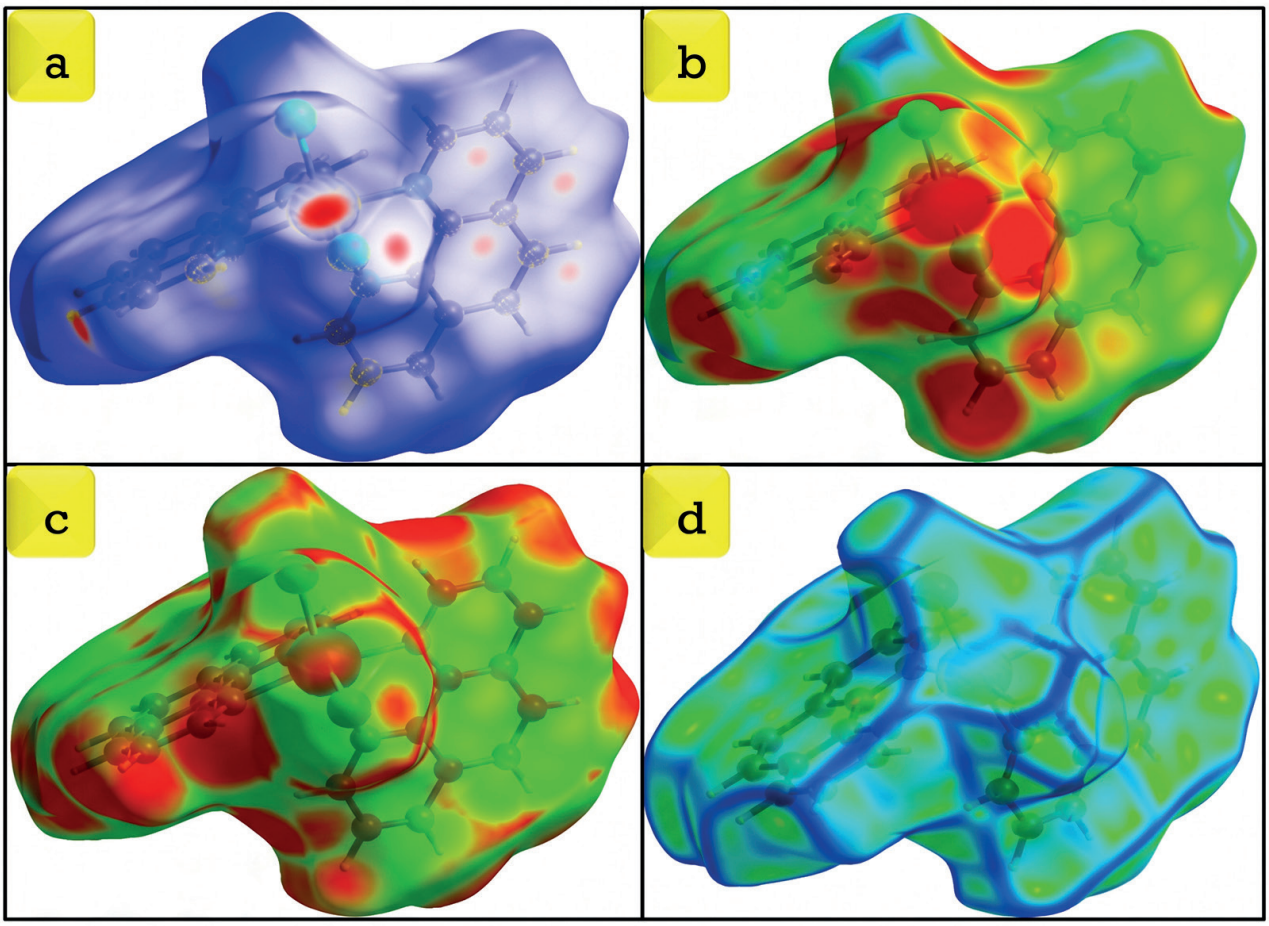



**Fig. 3**

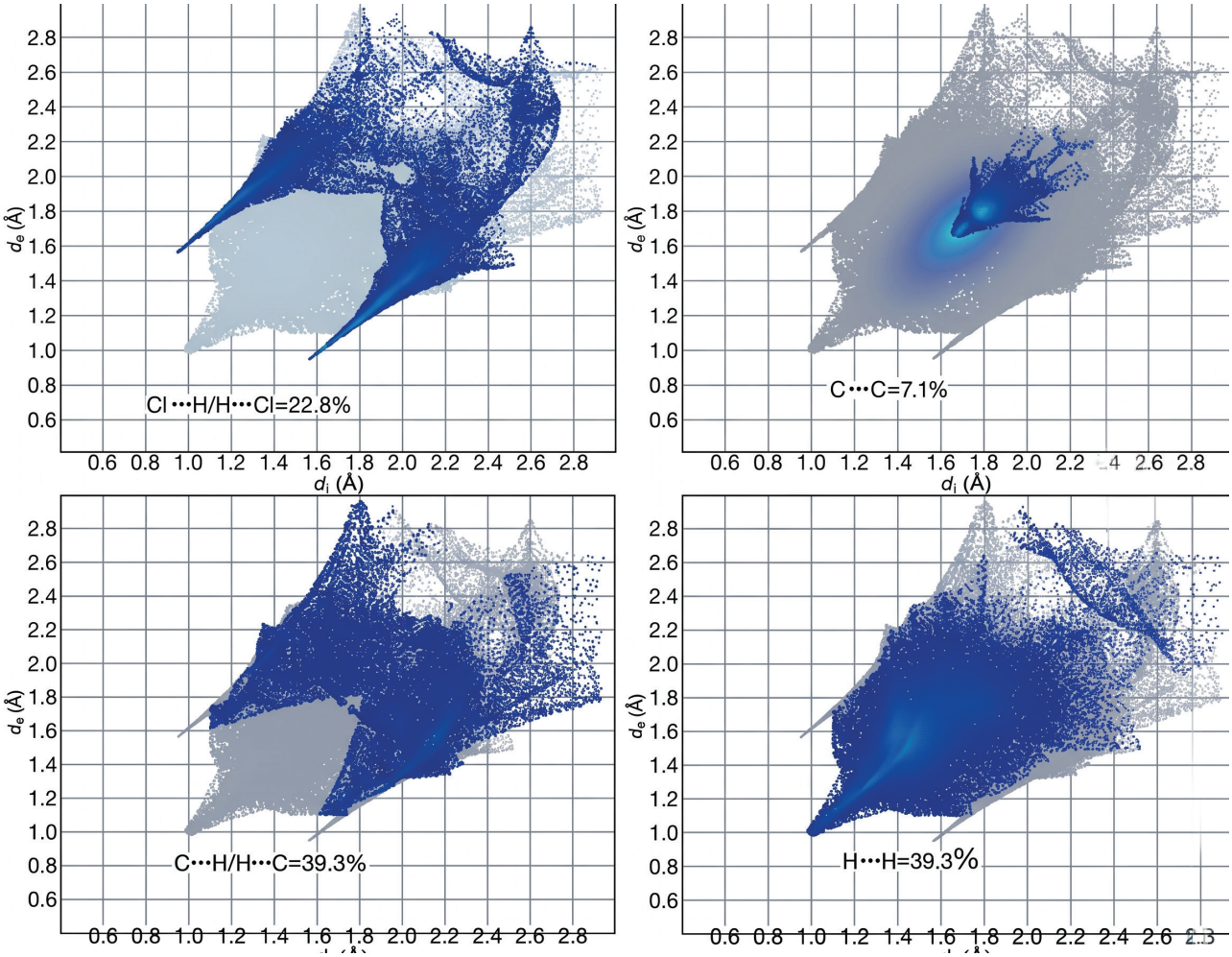
***Hirshfeld surface maps a)$d_{norm}$ (b) $d_e$ (c) $d_i$ and (d) cudvedness***

Maps of Hirschfeld surfaces based on the parameters $_{dnorm,}$ di, de and curvature were an important tool for determining the type of interatomic distances in the structure. The red zones observed on Dnorm maps represent short interatomic distances, i.e., strong interactions; white corresponds to neutral distances, and blue corresponds to relatively long contacts. The red regions observed in the analyzed structure are mainly located in the Cl···H/H···Cl regions, which indicates the strong electrostatic nature of the contacts. These interactions play an important stabilizing role in molecular packaging.

Fingerprint analysis allowed us to determine the quantitative fractions of contacts. According to the calculated results: H···H=39.3%, C···H/H···C=39.3%, Cl···H/H···Cl=22.8% and C···C=7.1%. The largest percentages correspond to contacts H···H and C···H/H···C . This indicates the predominance of van der Waals-type dispersion forces in the crystal lattice.

Fig.4

*Fingerprin plots*




These forces make a significant contribution to the overall mechanical and spatial stability of the structure, ensuring tight packing between molecules. Cl···H/H···Cl contacts (22.8%) represent polar hydrogen bonds. They form directed electrostatic interactions in the crystal lattice, stabilizing intermolecular equilibrium. On the contrary, a relatively low proportion of C···C contacts (7.1%) π-π indicates a limited stacking interaction, which reduces the vertical assembly of aromatic ring systems. Analysis of the curvature map showed the predominance of low-curvature surfaces, which confirms the presence of smooth intermolecular interfaces and dense molecular arrangement. At the same time, the maps $_{di}$ and $_{de}$ show that the intermolecular surface distances are in the optimal range, proving that the stability of the structure is ensured by a harmonious combination of dispersed forces and hydrogen bonds.[1]

## Conclusions

A new manganese(II) coordination complex, $[Mn(Phen)_2Cl_2]$, was successfully synthesised using 1,10-phenanthroline as the chelating ligand. Single-crystal X-ray diffraction (SCXRD) analysis established that the complex crystallises in the monoclinic crystal system, with the Mn(II) ion adopting a distorted octahedral coordination geometry formed by four nitrogen atoms from two 1,10-phenanthroline ligands and two chloride ions. Powder X-ray diffraction (PXRD) confirmed the phase purity and high crystallinity of the synthesised compound through the close agreement between the experimental and simulated diffraction patterns. Hirshfeld surface analysis provided valuable insight into the crystal packing, revealing that H···H, C···H/H···C, and Cl···H/H···Cl contacts are the dominant intermolecular interactions responsible for stabilising the crystal structure.

1 Mukimova, G. Z., Toshtemirov, A. E., & Saidov, D. K. (2022, January). Synthesis and study of coordination compound of cobalt and nickel succinate with urea. In *Conference XVII Numanov's Readings' Results of innovative research in the field of chemical and technical sciences in the XXI century'Proceedings* (No. INIS-TJ--031, pp. 97-99).