

CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS OF NICKEL (II) CHLORIDE WITH 1,3,4-THIADIAZOLE-2,5-DIAMINE

¹Ruziboyeva G.S., ²Turaev Kh.Kh., ³Ibragimov A.B., ¹Abdiyeva D.M
²Nazarov Y.E.

¹Denau Institute of Entrepreneurship and Pedagogy, Sharof Rashidov Street 360, ²Termiz State University, Barkamol Avlod Street, Termiz, ³Institute of General and Inorganic Chemistry, Academy of Sciences of Uzbekistan, Tashkent
E-mail: ruziboyevaguzal22@gmail.com

Abstract. *Background of the problem.* Synthesis and study of oxo-bridged trinuclear nickel (II) complex compounds is a relevant direction of modern coordination chemistry and is associated with the creation of materials with controlled structural and functional properties.

Objective: To synthesize oxo-bridged trinuclear compounds in the presence of new 1,3,4 thiodiazole 2,5 diamine and nickel (II) chloride and analyze its structural, morphological and spectroscopic properties.

Methodology: The Ni(II) coordination compound was structurally characterized by single-crystal X-ray diffraction, while the intermolecular interactions within the crystal lattice were systematically investigated using Hirshfeld surface analysis. *Scientific novelty.* A new complex compound with unique morphological and crystalline properties was synthesized.

Results: The structure and physicochemical properties of the synthesized new coordination compound were studied.

Keywords: Nickel-based oxo-bridged trinuclear complex compound, L1, X-ray, Hirshfeld surface.

Properties:

- The complex was synthesized in the presence of Ni(II) salt, L1, ethanol and water.
- It has a discrete structure.

Introduction.

Polynuclear transition-metal clusters have emerged as an important class of coordination compounds because of their diverse structural architectures and broad



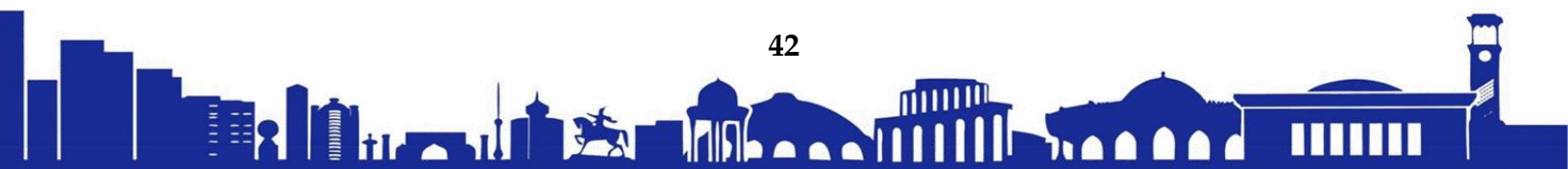
applications in catalysis, magnetic materials, materials chemistry, and bioinorganic systems [1]. Among these systems, oxo-bridged multinuclear assemblies are of particular interest because μ -oxo ligands effectively stabilize polynuclear frameworks and facilitate electronic communication between neighbouring metal centres, thereby resembling structural motifs found in metalloenzymes and functional metal-oxide materials [2-3]. Furthermore, the incorporation of a central oxo bridge generally enhances the structural rigidity of the cluster core and promotes cooperative metal–metal interactions, which are crucial for the physicochemical properties of multinuclear complexes [4].

Ligand design plays a decisive role in controlling nuclearity, geometry, and functional behaviour in polynuclear coordination compounds [5]. Nitrogen- and sulfur-donor heterocycles are especially effective for stabilizing multinuclear architectures due to their adaptable coordination modes and ability to promote secondary supramolecular interactions [7]. Among these ligands, thiadiazole derivatives have received increasing attention owing to their strong metal-binding ability and well-documented biological relevance. 1,3,4-Thiadiazole frameworks are known to exhibit pharmacological activity and have been widely explored as ligands for transition-metal complexes, with properties including antimicrobial, enzymatic, and therapeutic activities [8]. The 1,3,4-thiadiazole-2,5-diamine (TDAD) ligand is particularly attractive because it provides multiple nitrogen donor atoms while retaining terminal amino groups capable of forming intermolecular hydrogen bonds. These features enable the construction of robust multinuclear frameworks and promote extended supramolecular organization in the solid state [9].

In this context, the present study describes the synthesis and comprehensive characterization of an oxo-bridged trinuclear nickel(II) coordination cluster, trichlorido(μ_3 -oxo)hexakis(1,3,4-thiadiazole-2,5-diamine)trinickel(II) chloride, $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$. The complex features a symmetrically arranged Ni_3O core stabilized by six thiadiazole ligands, providing a rare example of a nitrogen-rich μ_3 -oxo-bridged trinuclear nickel framework that integrates structural analysis with physicochemical and antimicrobial evaluation. The structural and physicochemical properties were elucidated using single-crystal X-ray diffraction together with complementary analytical techniques.

Results and discussion.

Single-crystal X-ray diffraction analysis



Crystal Structure Determination

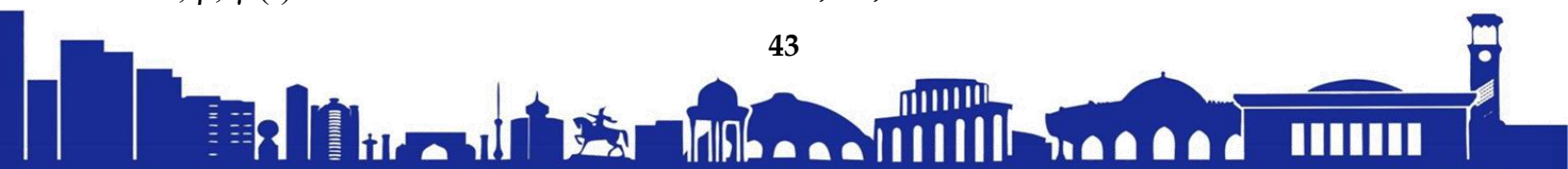
Single-crystal X-ray diffraction analysis confirmed the molecular and crystal structure of $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$. The crystallographic data collection and refinement parameters are summarized in Table 1. The complex crystallizes in the hexagonal crystal system with centrosymmetric space group $P6_3/mcm$ (No. 193) at 293 K. The unit-cell parameters are $a = b = 10.5430(2) \text{ \AA}$ and $c = 18.7330(4) \text{ \AA}$, giving a cell volume of $1803.29(8) \text{ \AA}^3$ with $Z = 12$. The structure refinement converged satisfactorily with final $R = 0.0477$ and $wR2 = 0.1364$, indicating good agreement between observed and calculated structure factors.

Asymmetric Unit and Molecular Structure

The asymmetric unit of the complex is shown in Fig. 1(a), with displacement ellipsoids drawn at the 35 % probability level. It comprises one Ni(II) centre coordinated by one μ_3 -oxo atom, four nitrogen atoms from four independent TDAD ligands, and one terminal chloride ion; positional disorder is observed for the amino nitrogen N(2) and its attached hydrogen atoms, which are modelled over two sites with partial occupancies (Fig. 2). The complete trinuclear molecular structure is illustrated in Fig. 1(b), revealing a centrosymmetric Ni_3O core in which a central μ_3 -oxo atom symmetrically bridges three Ni(II) ions [10].

Table 1. Crystal data and structure refinement for $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$.

CCDC	2518737
Formula	$\text{C}_2\text{H}_2\text{Cl}_{0.83}\text{N}_3\text{Ni}_{0.50}\text{O}_{0.17}\text{S}$
Formula Weight (g/mol)	161.69
Temperature(K)	293(2)
Wavelength	1.54184
Crystal size (mm^3)	0.17 x 0.14 x 0.14
Shape	Needle
Crystal System	Hexagonal
Space Group	$P6_3/mcm$ (No.193)
a, b, c ($\text{\AA}$)	10.5430(2), 10.5430(2), 18.7330(4)
α, β, γ ($^\circ$)	90, 90, 120



Volume ($\text{\AA}^3$)	1803.29(8)
Z	12
D (calc) [g/cm^3]	1.787
Mu [mm^{-1}]	8.851
F(000)	966
Index ranges	$-13 \leq h \leq 13, -12 \leq k \leq 12, -23 \leq l \leq 18$
Reflections collected	11319
Theta Min-Max [$^\circ$]	4.829, 75.581
Reflections with $I > 2(I)$	703 [R(int) = 0.0419]
Data/restraints/parameters	703/0/47
Goodness-of-fit on F^2	1.089
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0498, wR2 = 0.1409
R indices (all data)	R1 = 0.0515, wR2 = 0.1426

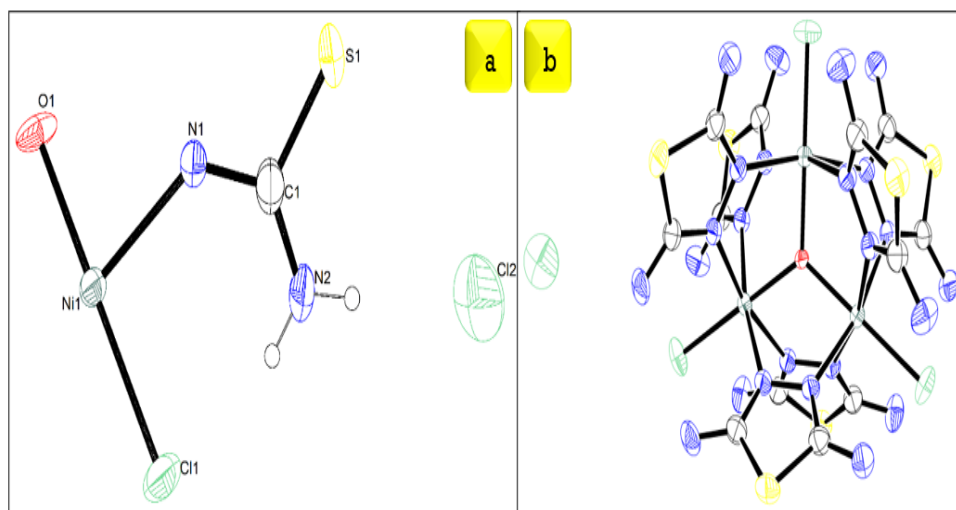
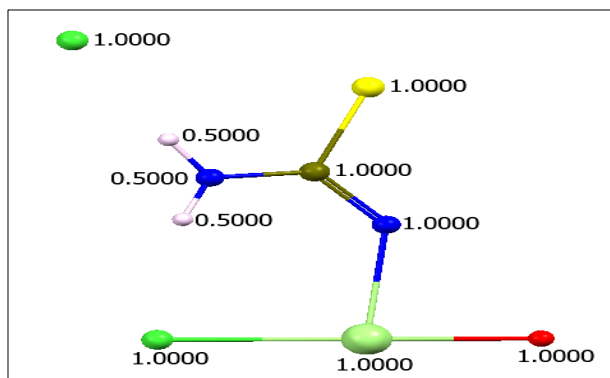


Fig. 1 (a) Asymmetric unit with atom numbering and displacement ellipsoids drawn at the 35% probability level; (b) ORTEP representation of the





Coordination Environment and Bond Geometry

Each Ni(II) centre exhibits a distorted octahedral coordination geometry, defined by an N_4OCl donor set. Selected bond lengths and angles are listed in Table 2. The Ni–O(μ_3 -oxo) bond distance of 1.9579(9) Å reflects strong metal-oxygen bonding, while the Ni–N bond lengths are narrowly distributed around 2.156 Å, indicating uniform coordination by the TDAD ligands. The terminal Ni–Cl bond length of 2.3494(19) Å falls within the expected range reported for monodentate chloride ligands in Ni(II) coordination complexes (typically ≈ 2.20 – 2.40 Å), consistent with previously described crystal structures of nickel(II) chloride-containing complexes [11]. The Ni–O–Ni angles are fixed at 120° , confirming a planar triangular arrangement of the Ni_3O core.

Fig. 2 Asymmetric unit of $[Ni_3O(TDAD)_6Cl_3]Cl$ with atoms labelled and occupancies indicated.

Table 2 The selected bond lengths (Å), angles ($^\circ$) and dihedral angles ($^\circ$) for $[Ni_3O(TDAD)_6Cl_3]Cl$

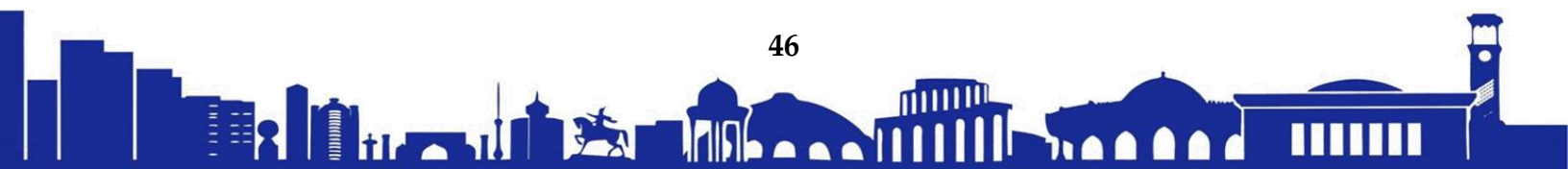
Bond	Length [Å]	Bond	Length [Å]
Ni(1)-Cl(1)	2.349(2)	S(1)-C(1)	1.723(4)
Ni(1)-O(1)	1.9577(10)	N(1)-N(1)	1.388(6)
Ni(1)-N(1)	2.155(3)	N(1)-C(1)	1.304(4)
Ni(1)-N(1)	2.155(3)	C(1)-N(2)	1.299(8)
Ni(1)-N(1)	2.155(3)	N(2)-H(2A)	0.86
Ni(1)-N(1)	2.155(3)	N(2)-H(2B)	0.86
S(1)-C(1)	1.723(4)		

Bond	Angle [°]	Bond	Angle [°]
O(1)-Ni(1)-Cl(1)	180.0	N(1)-Ni(1)-N(1)	93.69(14)
O(1)-Ni(1)-N(1)	83.38(8)	C(1)-S(1)-C(1)	86.9(3)
O(1)-Ni(1)-N(1)	83.37(8)	Ni(1)-O(1)-Ni(1)	120.000(1)
O(1)-Ni(1)-N(1)	83.37(8)	Ni(1)-O(1)-Ni(1)	120.0
O(1)-Ni(1)-N(1)	83.37(8)	Ni(1)-O(1)-Ni(1)	120.0
N(1)-Ni(1)-Cl(1)	96.63(8)	N(1)-N(1)-Ni(1)	117.69(8)
N(1)-Ni(1)-Cl(1)	96.63(8)	C(1)-N(1)-Ni(1)	130.2(3)
N(1)-Ni(1)-Cl(1)	96.63(8)	C(1)-N(1)-N(1)	112.1(2)
N(1)-Ni(1)-Cl(1)	96.62(8)	N(1)-C(1)-S(1)	114.4(3)
N(1)-Ni(1)-N(1)	84.78(14)	N(1)-C(1)-N(2)	119.3(4)
N(1)-Ni(1)-N(1)	166.75(16)	N(2)-C(1)-S(1)	126.3(5)
N(1)-Ni(1)-N(1)	84.78(14)	C(1)-N(2)-H(2A)	120.0
N(1)-Ni(1)-N(1)	93.69(14)	C(1)-N(2)-H(2B)	120.0
N(1)-Ni(1)-N(1)	166.75(16)	H(2A)-N(2)-H(2B)	120.0
Dihedral bond	Angle [°]	Dihedral bond	Angle [°]
Ni(1)-N(1)-C(1)-S(1)	178.76(17)	N(1)-N(1)-C(1)-N(2)	179.0(6)
Ni(1)-N(1)-C(1)-N(2)	-1.3(8)	C(1)-S(1)-C(1)-N(1)	1.2(4)
N(1)-N(1)-C(1)-S(1)	-1.0(3)	C(1)-S(1)-C(1)-N(2)	-178.7(5)

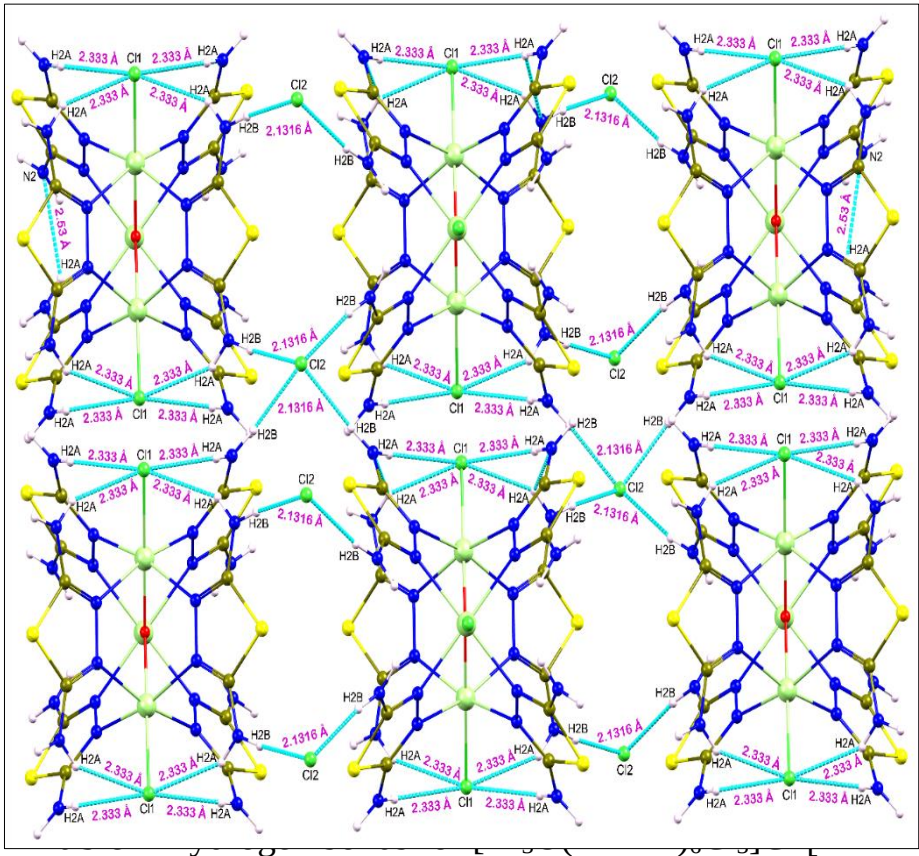
Symmetry transformations used to generate equivalent atoms:.

Hydrogen-Bonding Interactions

In addition to coordination bonds, extensive hydrogen bonding contributes to the stabilization of the crystal structure. The hydrogen-bonding network is illustrated in Fig. 3, and the corresponding geometric parameters are summarized in Table 2. The amino groups of the TDAD ligands act as hydrogen-bond donors, forming N-H $\cdots$ Cl interactions with both coordinated and lattice chloride ions, as well as weaker N-H $\cdots$ N contacts between adjacent ligands. The short H $\cdots$ Cl distances (2.1316-2.333 Å) and near-linear D-



H⋯A angles (up to 170.9°) indicate relatively strong hydrogen bonds that link neighbouring trinuclear units into extended supramolecular assemblies.



D-H⋯A	Fig. 3	The hydrogen bonding network of [Ni ₃ O(TDA) ₆ Cl ₃]·Cl	d(D-H)	d(H⋯A)	d(D⋯A)	<(DHA)
N(2)-H(2A)⋯Cl(1)			0.86	2.333	3.093	147.5
N(2)-H(2A)⋯N(2)			0.86	2.556	3.124(2)	124.5
N(2)-H(2B)⋯Cl(2)			0.86	2.131	2.983	171.2

Symmetry transformations used to generate equivalent atoms:

Comparative structural analysis and supramolecular features

To place the structure of the present trinuclear cluster in context, a comparison with representative Ni(II) complexes retrieved from the CCDC database [41-46] was performed. The selected literature structures crystallize in various crystal systems but consistently display distorted octahedral Ni(II) coordination environments with typical Ni–N distances of approximately 2.02-2.08 Å, Ni–O distances near 2.03–2.13 Å, and Ni–

Cl separations around 2.36-2.40 Å. In contrast, the present compound $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$ exhibits slightly longer Ni–N bonds (≈ 2.155 Å) together with a notably shorter Ni–O bond (≈ 1.958 Å), reflecting the strong coordination of the oxo donor within the trinuclear framework. While most reported structures are mononuclear species stabilized primarily by conventional hydrogen bonding and π - π stacking, the present structure contains a multinuclear Ni_3O core that generates a distinct coordination topology and extended hydrogen-bond-assisted supramolecular assembly. Further insight into intermolecular stabilization was obtained from hydrogen-bond comparisons (Table 3). The literature complexes typically show networks dominated by N-H $\cdots$ Cl and O-H $\cdots$ Cl interactions, often supplemented by weaker C-H $\cdots$ Cl contacts. A similar pattern is observed in the present compound, where multiple N-H donors from the TDAD ligands participate in hydrogen bonding with chloride acceptors, forming a three-dimensional supramolecular framework. Taken together, these comparisons demonstrate that although the local coordination geometry around Ni(II) remains octahedral, the present compound is structurally distinguished by its trinuclear oxo-bridged core and the resulting multidirectional hydrogen-bonding architecture, which collectively define the structural novelty of the reported system.

Table 3. Selected hydrogen-bond parameters (Å, °) for representative Ni(II) complexes (CCDC entries) and the present complex, showing key D-H $\cdots$ A intermolecular contacts governing supramolecular packing.

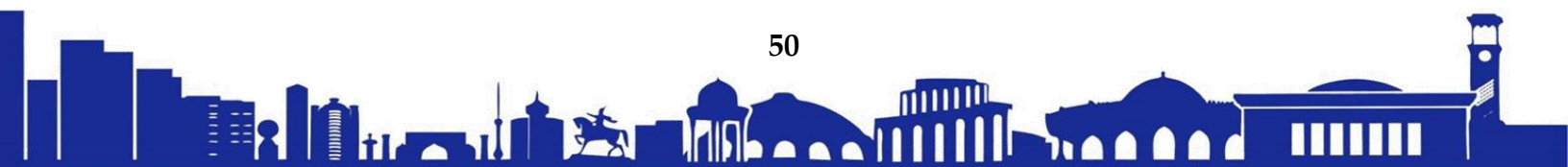
D-H $\cdots$ A	d(D-H)	d(H $\cdots$ A)	d(D $\cdots$ A)	<(DHA)
OYOLOG (2034867)				
N2-H2N $\cdots$ O9	0.85(2)	1.94(2)	2.783(3)	171(3)
N4-H4N $\cdots$ O10	0.86(3)	2.01(3)	2.865(8)	173(5)
O5-H5O $\cdots$ Cl2	0.84(2)	2.28(2)	3.0922(19)	163(3)
N6-H6N $\cdots$ Cl1	0.86(2)	2.41(2)	3.250(2)	166(2)
O6-H6O $\cdots$ Cl4	0.84(2)	2.20(2)	3.020(2)	166(3)
O7-H7O $\cdots$ Cl1	0.83(2)	2.264(18)	3.070(2)	164(3)
N8-H8N $\cdots$ Cl1	0.83(3)	2.43(3)	3.234(2)	162(3)
O8-H8O $\cdots$ Cl3	0.84(3)	2.18(3)	3.006(2)	173(3)
O9-H9O $\cdots$ Cl4	0.83(3)	2.31(3)	3.125(2)	167(3)

O10-H10O...Cl2	0.84(5)	2.54(5)	3.374(3)	173(5)
C16-H16B...Cl3	0.99	2.61	3.349(7)	132
C20-H20...Cl2	0.95	2.67	3.537(3)	153
C33-H33B...Cl3	0.98	2.78	3.679(3)	154
IFOYAG (1406344)				
O1WA-H1W2...Cl1	0.82(3)	2.38(3)	3.1684(13)	164(2)
O1WA-H1W1...Cl2	0.84(3)	2.26(3)	3.0919(14)	171(2)
O1WB-H1W4...Cl1	0.84(3)	2.26(3)	3.0679(15)	165(3)
C2B-H2BA...Cl1	0.95	2.79	3.461(2)	128.00
TOLTOE (686886)				
N1-H5...Cl1	0.87	2.52	3.331(2)	155
O1-H10...Cl1	0.85	2.19	3.0320(19)	170
C3-H2...Cl1	0.94	2.74	3.552(3)	144
HIBYOJ (1826295)				
O5-H1O5...Cl3	0.79(2)	2.25(2)	3.0299(18)	167(3)
O6-H1O6...Cl1	0.80(2)	2.19(2)	2.979(2)	169(2)
N2-H2A...Cl2	0.88	2.7000	3.520(2)	156
O7-H1O7...Cl4	0.796(13)	2.240(14)	3.0223(14)	168(2)
O8-H1O8...Cl2	0.80(2)	2.25(2)	3.0268(16)	165(2)
N6-H6A...Cl4	0.88	2.77	3.550(2)	149
N8-H8A...Cl3	0.88	2.62	3.477(2)	165
N8-H8B...Cl3	0.88	2.48	3.336(2)	164
C9-H9...Cl1	0.95	2.79	3.503(2)	133
UYOJIC (847181)				
O6-H6C...Cl3	0.86(3)	2.22(3)	3.057(3)	167(3)
O6-H6D...O9	0.86(3)	1.96(3)	2.797(5)	167(3)
O7-H7A...Cl1	0.85(3)	2.32(3)	3.139(3)	163(4)
O7-H7B...Cl4	0.85(3)	2.45(3)	3.292(2)	169(3)
O8-H8A...Cl2	0.84(3)	2.27(3)	3.104(2)	173(3)
O8-H8B...Cl3	0.84(2)	2.37(3)	3.167(2)	159(2)

O9-H9A...Cl2	0.86(3)	2.44(3)	3.163(3)	142(4)
O9-H9B...Cl1	0.86(4)	2.33(4)	3.173(4)	170(4)
C2-H2...Cl4	0.93	2.67	3.520(4)	153
POXNOJ (1055581)				
N2-H2A...Cl1	0.86	2.5	3.277(2)	150
[Ni₃O(TDAD)₆Cl₃]Cl				
N(2)-H(2A)...Cl(1)	0.86	2.333	3.09	147.1
N(2)-H(2A)...N(2)	0.86	2.53	3.10(2)	124.7
N(2)-H(2B)...Cl(2)	0.86	2.1316	2.984	170.9

Hirshfeld surface analysis.

Hirshfeld surface analysis was employed to examine and quantify the intermolecular interactions that govern the crystal packing of $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$, providing a three-dimensional visualization of contact regions between neighbouring molecular units (Fig. 4). Mapping the Hirshfeld surface over the internal distance parameter (d_i) highlights close contacts involving atoms located within the surface. In this representation (Fig. 4(a)), distinct features are observed near hydrogen atoms bonded to nitrogen, indicating their proximity to electronegative neighbouring atoms. These features reflect the prominent donor behaviour of the amino groups of the TDAD ligands, which actively participate in hydrogen-bond formation. The external distance (d_e) surface (Fig. 4(b)), which emphasizes interactions with atoms outside the Hirshfeld surface, reveals pronounced regions corresponding to chloride and sulfur atoms. These regions illustrate the strong acceptor character of chloride ions and the participation of sulfur atoms from the thiadiazole rings in intermolecular contacts. The complementary nature of the d_i and d_e surfaces confirms the directional hydrogen bonding between N-H donors and chloride acceptors, as well as secondary contacts involving sulfur. The normalized contact distance (d_{norm}) surface (Fig. 4(c)) provides a comprehensive overview of the strength and significance of intermolecular interactions using a colour scale ranging from negative to positive values [12-14].



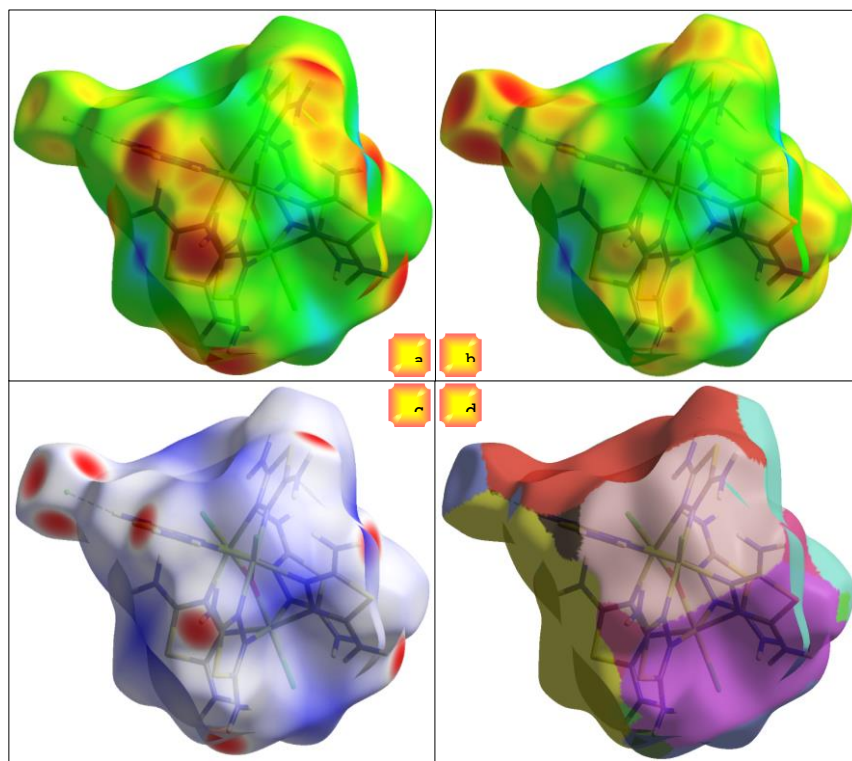
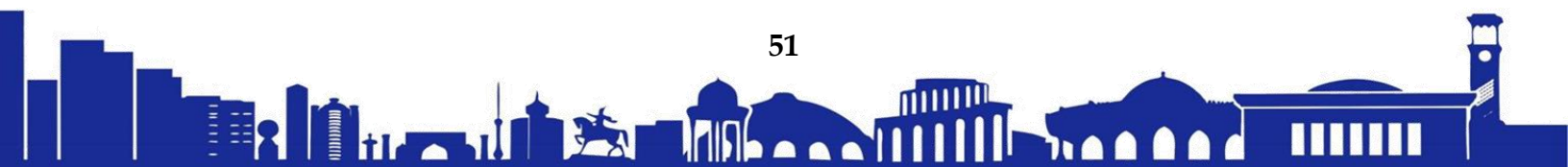


Fig. 4 Hirshfeld surface representations of $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$: (a) d_i map, (b) d_e map, (c) d_{norm} map and (d) fragment patch map.

Intense red spots appear in regions where intermolecular separations are shorter than the sum of van der Waals radii, indicating strong contacts. These red regions are predominantly localized around chloride ions and hydrogen atoms of the amino groups, clearly identifying $\text{N-H}\cdots\text{Cl}$ hydrogen bonds as the dominant stabilizing interactions within the lattice. White areas correspond to contacts close to van der Waals separations, while blue regions

represent longer, less influential interactions. The fragment patch representation (Fig. 4(d)) further partitions the Hirshfeld surface according to neighbouring molecular fragments. Distinct and well-defined patches surrounding chloride ions and thiadiazole rings indicate specific, directional interactions, whereas broader patches are associated with diffuse van der Waals contacts. Together, these surface features demonstrate that the crystal packing is primarily controlled by hydrogen bonding centred on chloride ions, reinforced by additional heteroatom-based interactions that collectively generate a robust three-dimensional supramolecular framework.

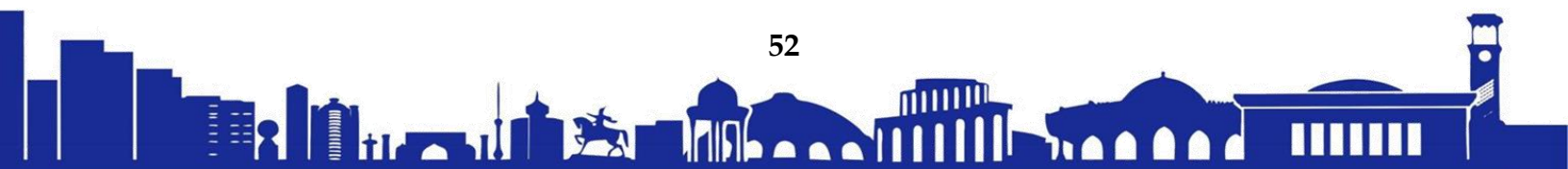
Conclusion. A new oxo-bridged trinuclear nickel(II) coordination cluster, $[\text{Ni}_3\text{O}(\text{TDAD})_6\text{Cl}_3]\text{Cl}$, supported by 1,3,4-thiadiazole-2,5-diamine ligands, was successfully synthesized and comprehensively characterized. Single-crystal X-ray diffraction analysis revealed the formation of a centrosymmetric trinuclear Ni_3O core in which each $\text{Ni}(\text{II})$ centre adopts a distorted octahedral coordination geometry. The



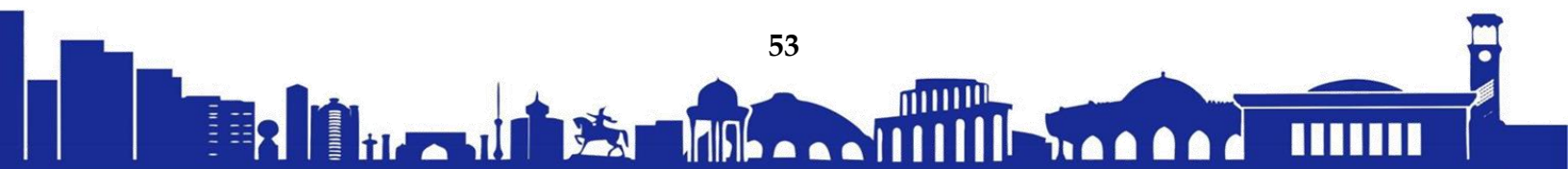
structural study demonstrated that the μ_3 -oxo bridge plays a crucial role in stabilizing the trinuclear framework and promoting cooperative metal–metal interactions within the cluster core. Extensive intermolecular N-H $\cdots$ Cl and N-H $\cdots$ N hydrogen-bonding interactions further contribute to the stabilization of the crystal packing, generating a robust three-dimensional supramolecular architecture. Hirshfeld surface analysis confirmed that hydrogen-bonding interactions involving chloride ions represent the dominant intermolecular contacts governing crystal packing stabilization. Comparative analysis with related CCDC-reported Ni(II) complexes demonstrated that the present compound is structurally distinguished by its trinuclear oxo-bridged topology and multidirectional supramolecular interaction network. Overall, the obtained results expand the structural chemistry of nitrogen-rich oxo-bridged nickel(II) clusters and provide valuable insight into the relationship between coordination geometry and supramolecular organization in multinuclear transition-metal systems.

References

- [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. Mamatkodiroy, 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] J.A. Alonso, Electronic and atomic structure and magnetism of transition-metal clusters, Chem. Rev. 100 (2000) 637–678. <https://doi.org/10.1021/cr980391o>.
- [3] J. Tang, L. Zhao, Polynuclear organometallic clusters: synthesis, structure, and reactivity studies, Chem. Commun. 56 (2020) 1915–1925. <https://doi.org/10.1039/C9CC09354K>.
- [4] D.A. Kuznetsov, T.A. Bazhenova, I.V. Fedyanin, V.M. Martynenko, A.F. Shestakov, G.N. Petrova, N.Y.S. Komarova, Tri-, tetra- and hexanuclear mixed-valence molybdenum clusters: structural diversity and catalysis of acetylene hydrogenation, Dalton Trans. 45 (2016) 16309–16316. <https://doi.org/10.1039/C6DT02965E>.
- [5] S.P. Misra, A. Ranjan, R. Shrimali, P.A. Deshpande, Strategies for rational design and applications of transition metal clusters, Chem. Phys. Rev. 5 (2024) 031301. <https://doi.org/10.1063/5.0204606>.



- [6] A. Bencini, S. Midollini, Some synthetic and theoretical aspects of the chemistry of polynuclear transition-metal complexes, *Coord. Chem. Rev.* 120 (1992) 87–136.
[https://doi.org/10.1016/0010-8545\(92\)80048-V](https://doi.org/10.1016/0010-8545(92)80048-V).
- [7] 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>
- [8] TK, K., & Ibragimov, A. B. (2025). structural analysis of a mixed-ligand coordination polymer with Cd (II) based on 1-hydroxy-2-naphthoic and acetic acids. *Journal of Universal Science Research*, 3(5), 120-122.
- [9] TURAEV, K., IBRAGIMOV, A., SAIDOV, D., XOLTO‘RAYEV, Q. B., & NURULLAEVA, Z. (2025). OBTAINING CRYSTALLINE STRUCTURE AND THERMAL PROPERTIES OF A NEW MIXED-LIGAND COORDINATION POLYMER OF MAGNESIUM. *Uzbek Chemical Journal/O'zbekiston Kimyo Jurnali*, (3).
- [10] TURAEV, K., IBRAGIMOV, A., SAIDOV, D., TURSUNOV, B., RUZIYEV, U., & NURULLAEVA, Z. (2025). STRUCTURE AND PROPERTIES OF A MIXED-LIGAND COORDINATION POLYMER SYNTHESIZED FROM 3,5 DIMETHYLPYRAZOLE, FUMARIC ACID, AND COBALT (II) CHLORIDE HEXAHYDRATE. *Uzbek Chemical Journal/O'zbekiston Kimyo Jurnali*, (3).
- [11] Saidov, D. X., & Turayev, X. X. AB Ibragimov coordination polymer based on 1-hydroxy 2-naphthoic acid and Cd (CH₃COO)₂ · 2H₂O//republican scientific and practical conference on the topic:“creating national aspects for patriotic education of military-academic lyceum students and implementing modern educational trends” Articles of the Republican scientific and practical conference, Termez, April 18, 2025 XX To ‘rayev, AB Ibragimov, DX Saidov, B.Ch. Tursunov, RU Ro ‘ziyev, ZV Nurullayeva.
- [12] SAIDOV, D., TURAEV, K., IBRAGIMOV, A., MUKUMOVA, G., TOIROVA, G., & NURULLAEVA, Z. (2025). SYNTHESIS AND COMPREHENSIVE CHARACTERIZATION OF A Cd (II) COORDINATION POLYMER BASED ON



- 1-HYDROXY-2-NAPHTHOIC ACID. *Uzbek Chemical Journal/O'zbekiston Kimyo Jurnali*, (6).
- [13] SAIDOV, D., TURAEV, K., IBRAGIMOV, A., RUZIEV, U., KHOLTURAEV, K., & GANIEVA, S. (2025). STRUCTURE, THERMODYNAMIC STABILITY, AND CONDUCTIVITY OF A Cd (II) COORDINATION POLYMER BASED ON HNA. *Uzbek Chemical Journal/O'zbekiston Kimyo Jurnali*, (6).
- [14] TURAEV, K., IBRAGIMOV, A., SAIDOV, D., TURSUNOV, B., RUZIYEV, U., & NURULLAEVA, Z. (2025). STRUCTURE AND PROPERTIES OF A MIXED-LIGAND COORDINATION POLYMER SYNTHESIZED FROM 3,5-DIMETHYLPYRAZOLE, FUMARIC ACID, AND COBALT (II) CHLORIDE HEXAHYDRATE. *Uzbek Chemical Journal/O'zbekiston Kimyo Jurnali*, (3).
- [15] Mukimova, G. Z., Toshtemirov, A. E., & Saidov, D. K. (2022, January). Synthesis and study of the 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).

¹Рузибоева Г.С., ²Тураев Х.Х., ³Ибрагимов А.Б. ¹Абдиева Д.М
²Назаров Ю.Э.

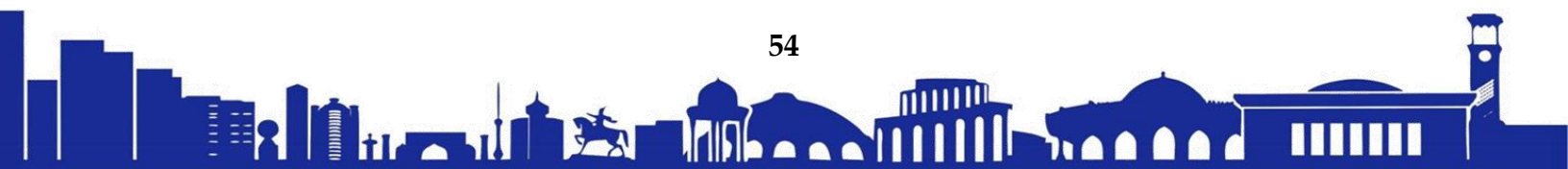
КРИСТАЛЛИЧЕСКАЯ СТРУКТУРА И АНАЛИЗ ПОВЕРХНОСТИ ХИРШФЕЛЬДА КОМПЛЕКСА ХЛОРИДА НИКЕЛЯ (II) С 1,3,4- ТИАДИАЗОЛ-2,5-ДИАМИНОМ

¹ Институт предпринимательства и педагогики Денау, Шароф улица Рашидова,
360, ²Термезский государственный университет, ул. Баркамол авлод, Термез.

³Институт общей и неорганической химии Академии наук Узбекистана,
Ташкент.

E-mail: ruziboyevaguzal22@gmail.com

Реферат. Предпосылки проблемы. Синтез и изучение оксо-мостовых
трехъядерных комплексов никеля(II) является важной областью современной



координационной химии, связанной с созданием материалов с контролируемыми структурными и функциональными свойствами.

Цель: Синтез нового оксо-мостового трехъядерного 1,3,4-тиодиазол-2,5-диамина в присутствии хлорида никеля(II) и анализ его структурных, морфологических и спектроскопических свойств.

Методология: Координационное соединение Ni (II) структурно характеризовалось монокристаллической рентгеновской дифракцией, а межмолекулярные взаимодействия в кристаллической решетке систематически изучались с помощью поверхностного анализа Гиршфельда. Научная новизна. Было синтезировано новое комплексное соединение с уникальными морфологическими и кристаллическими свойствами.

Научная новизна: Синтезировано новое сложное соединение с уникальными морфологическими и кристаллическими свойствами.

Полученные данные: Были изучены структура и физико-химические свойства вновь синтезированного координационного соединения.

Ключевые слова:

Никелевый оксо-мостовой трехъядерный комплексный материал, L1, Рентген, Анализ поверхности Хиршфельда.

Характеристики:

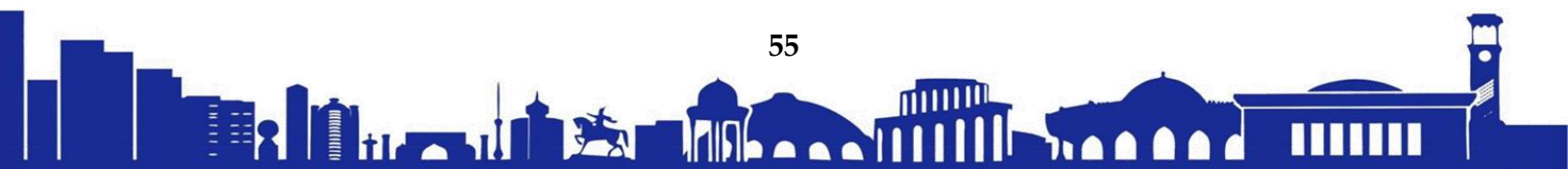
- Комплекс был синтезирован в присутствии соли Ni(II), L1, этанола и воды.
- Он имеет дискретную структуру.

¹Ruziboyeva G.S., ²Turayev X.X., ³Ibragimov A.B. ¹Abdiyeva D.M.,
²Nazarov Y.E.

**1,3,4-TIADIAZOL-2,5-DIAMIN BILAN NIKEL (II) XLORIDNING KRISTALL
TUZILISHI VA HIRSHFELD SIRTİ TAHLILI**

¹Denov tadbirkorlik va pedagogika instituti, Sharof Rashidov ko'chasi, 360-uy, ²Termiz davlat universiteti, Termiz sh., Barkamol avlod ko'chasi, ³O'zbekiston Fanlar akademiyasi Umumiy va noorganik kimyo instituti, Toshkent shahri

E-mail:ruziboyevaguzal22@gmail.com



Referat. *Muammoning kelib chiqishi.* Okso-ko'priqli uch yadroli nikel (II) kompleks birikmasini sintez qilish va o'rganish zamonaviy koordinatsion kimyoning dolzarb yo'nalishi bo'lib, tuzilma va funksional xususiyatlari boshqariladigan materiallar yaratish bilan bog'liq.

Maqsad: Yangi 1,3,4 tiodiazol 2,5 diamin va nikel(II) xlorid ishtirokida okso-ko'priqli uch yadroli sintez qilish hamda uning tuzilma, morfologik va spektroskopik xususiyatlarini tahlil qilish.

Metodologiya: Ni (II) koordinatsion birikmasi strukturaviy jihatdan monokristall rentgen difraksiyasi bilan tavsiflangan, kristall panjarasidagi molekulalararo o'zaro ta'sirlar esa Xirshfeld sirt tahlili yordamida tizimli ravishda o'rganilgan. Ilmiy yangilik. O'ziga xos morfologik va kristall xossalarga ega bo'lgan yangi kompleks birikma sintez qilindi.

Ilmiy yangiligi. O'ziga xos morfologik va kristall xususiyatlarga ega bo'lgan yangi kompleks birikma sintez qilindi.

Olingan natijalar: Sintez qilingan yangi koordinatsion birikmaning tuzilishi va fizik-kimyoviy xususiyatlari o'rganildi.

Kalit so'zlar: Nikel asosidagi okso-ko'priqli uch yadroli kompleks birikma, L1, X-Ray, Hirshfeld sirt tahlili.

Xususiyatlari:

- Kompleks Ni (II) tuzi, L1, etanol va suv ishtirokida sintez qilindi.
- Diskret tuzilishga ega.

