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Synthesis, Jahn-Teller labeled *via* crystal structure in *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex: S9/S6/C-H…O synthons, thermal, physicochemical and 1BNA-docking

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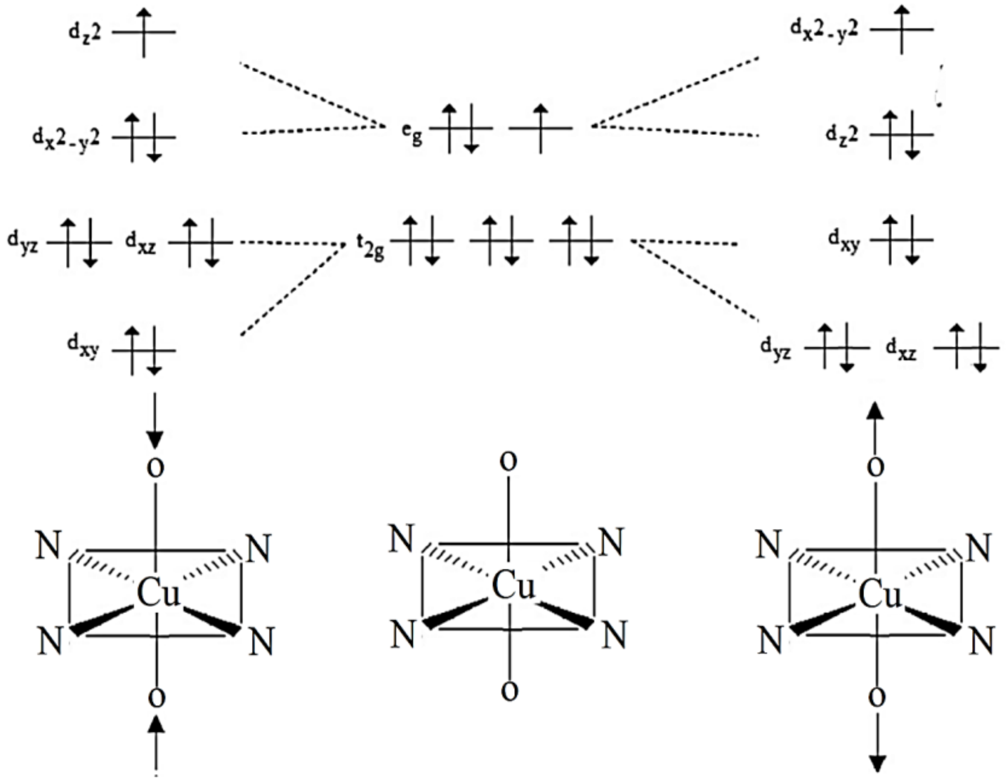
Abstract

The synthesis of the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex (where $Me_2N\text{-}Py$= N,N-dimethylpyridin-4-amine ligand) in significant yield involved the reaction of excess $Me_2N\text{-}Py$ ligand with $Cu(ClO_4)_2{\cdot}6H_2O$ in MeOH solvent. The progression of the complex synthesis was monitored by UV–Vis, FT-IR, EDX, XRD, MS, SEM, CHN-EA, and TG/DTG. The resulting complex crystallized in the Triclinic space $P\bar{1}$. In the solid state, the desired complex structure discrete a neutral *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ formula, with copper(II) adopting a distorted octahedral environment formed by four $Me_2N\text{-}Py$ ligands occupying the square planar position $Cu(Py)_4$, meanwhile, the two ClO_4 are in linear *trans*-position. The XRD measurements proved the existence of elongation Jahn-Teller distortion in the synthesized complex. Furthermore, a comprehensive analysis of the desired complex, including. XRD/HSA interactions revealed the presence of two S9 and S6 main 2D-synthons primarily formed through $C_{ph}\text{-}H\ldots.O_{ClO3}$ and $C_{Me\text{-}}H\ldots O_{ClO3}$ non-classical H-bonding interactions. Thermal stability assessments through TG/DTG indicated that the complexes with the most stable behavior underwent two degradation steps. The molecular docking of the desired complex against 1BNA-DNA was also evaluated.

Keywords: $[Cu(Py)_4]$, XRD/HSA, docking, Jahn-Teller, thermal.

1. Introduction

Several inorganic chemists have designed octahedral copper(II) complexes using monodentate ligands obtained from pyridine derivatives [1–6]. The redox characteristics of Cu(II) complexes have been thoroughly evaluated because of their biological relevance to imitateprotein functions [7–19]. [Copper(II)/Py]/[Copper(II)/phen] and their derivative complexes are of great importance among these complexes because of their flexibility to alter structurally and their wide range as DNA-binding, antibacterial, and COX/LOX-inflammation [20-23]. Supramolecular interactions, such as π-π stacking and hydrogen bonding, are essential in crystal engineering as they enable precise molecular recognition and facilitate the self-assembly of distinct supramolecular synthons [15]. Octahedral Cu(II) complexes with d^9 centres are commonly recognized to have the ability to display a Jahn-Teller distortion. This distortion is made possible by the existence of unpaired electrons located in the d-orbital. In the theorem of Jahn–Teller, the degeneracy in the orbitals (d-orbitals spin-splitting) results in a simultaneous compression or elongation along one Z-axis as in Scheme 1, which depicts the resultant trans-O_2CuN_4 complex electrical configuration. It is common practice to investigate these complexes' structures and any Jahn-Teller effect distortions using experimental methods including X-ray crystallography and spectroscopy.



Scheme 1. The elongation/compression Jahn–Teller diagram in *the trans*-O_2CuN_4 complex.

Molecular docking is a powerful tool for understanding the interaction between organic/inorganic material and DNA or enzymes. By utilizing non-covalent interactions, several studies offer vital insights into the mechanism of action by inserting a molecule at the binding site of a specific area on DNA or enzyme [24]. The utilization of in silico computational docking methods is crucial in the development of novel inorganic chemotherapeutic complexes that mimic the cisplatin drug. In silico docking analysis of various structural complexes enabled the exploration of energy, hydrogen bonding, and hydrophobic interactions, assisting in developing chemical therapies or understanding the behaviours of proposed drugs before they are introduced into biological cells.

This study details the synthesis of the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex utilizing 4-dimethylaminopyridine ligands. An XRD analysis was performed to confirm the presence of the distorted octahedral elongated Jahn-Teller complex. The HSA-compoution and exp. XRD reflected the excistence of 1 and 2D-synthons stabilized mainly by C-H…OCl H-bonds. In addition, various physicochemical and thermal analyses were employed to demonstrate the intricate structure. Subsequently, the complex was assessed using in silico molecular docking utilizing 1BNA-DNA.

2. Experimental analysis

2.1. Chemical and Physical analyses

The Elementar Varrio EL analyzer was employed solely for comprehensive CHN microanalysis. The acquisition of the FT-IR spectra involved the utilization of a spectrophotometer manufactured by 621-Perkin-Elmer. The UV-Vis spectra measurements are obtained using a spectrophotometer manufactured by 4060-LKB-Biochrom. The MS analysis was performed with a ThermoScientific-TM TSQ-Altis-TM Triple Quadrupole Mass Spectrometer. Sigma–Aldrich provided the necessary quantity of solvents and compounds and TG analysis were recorded via TGA-7 PerkinElmer.

2.2. Preparation of trans-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$

0.5 g (1.34 mmol) of $Cu(ClO_4)_2\cdot 6H_2O$ were dissolved in 30 ml of EtOH, and then 4 equivalents of N,N-dimethylpyridin-4-amine were added to the mixture. The reaction was performed in a closed system and stirred for 60 minutes until the blue colour transitioned into a greenish-blue. Subsequently, the reaction mixture was evacuated to a final volume of ~ 2 ml, and 40 ml of diethyl ether was added to cause the desired complex to precipitate. Following filtration, the resultant complex was extensively rinsed with 40 ml of CH_2Cl_2, yielding 83%.

2.2.1. ***Trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$**: MS m/z 751.2 $[M^+]$ (theo. 752.4), m.p. = 308.5 °C, molecular formula $C_{28}H_{40}Cl_2CuN_8O_8$ Cal: C, 44.77; H, 5.37; and N, 14.92%. Found C, 44.51; H, 5.22; N, 14.87%, IR (νcm^{-1}): 3052 ($\nu_{C\text{-}H}$ of py), 2960-2840($\nu_{C\text{-}H}$ of Me), 1555 ($\nu_{N=C}$), 510-680 ($\nu_{Cu\text{-}N}$) and ($\nu_{Cu\text{-}O}$), and 1092 (ν_{ClO4}), UV–Vis in MeOH: λ_{max} (ε/M^{-1}cm^{-1}): 277 nm (1.2×10^4) and 698 nm (8.2×10^2).

2.3. HSA and XRD determinations

The HSA study was conducted utilizing CrystalExplorer 17.1 [24]. The X-ray intensity data collection of the synthesized copper metal complex was conducted using graphite monochromatized Mo-Kα radiation (λ=0.7107 Å). The complex's structure is determined using the intrinsic phasing approach, namely the SHELXT [25]. The refining process is carried out in Olex2 using SHELXL-2015, utilizing least-squares minimization against F2 [26]. The non-hydrogen atoms were identified in the structures using different Fourier maps, and their anisotropic thermal characteristics were revised. The hydrogen atoms were immobilized in a fixed geometric arrangement and refined using the riding model. The maximum positive value of the complex number in the final Fourier difference map is 0.547 eÅ^{-3}. The crystallographic data and the refinement details are provided in Table 1.

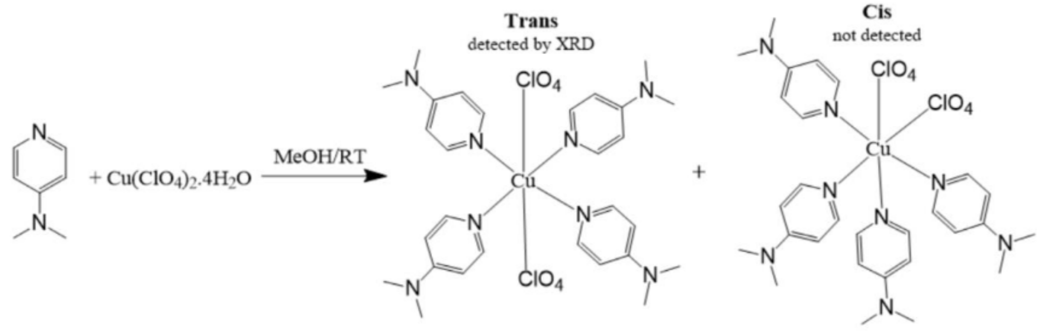
Table 1. *Trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ crystal data.

Empirical formula	$C_{28}H_{40}Cl_2CuN_8O_8$
Formula weight	751.12
Temperature (K)	293
Wavelength	0.71073
Crystal system, Space group, Z	Triclinic, *P*1, 4
$a/b/c$ (Å)	11.059(4)/16.743(6)/20.251(7)
α/β/γ (°)	97.360(5)/104.087(16)/102.733(8)
Volume (Å^3)	3481(2)
ρ_{calc}, Mg/cm^3	1.433
Absorption coefficient (μ/mm^{-1})	0.839
F(000)	1564
2θ range for data collection (°)	3.10 to 23.00
Index ranges	$-12 \le h \le 10$, $-18 \le k \le 18$, $-22 \le l \le 22$
Reflections collected	13810
Independent reflections	9589
Refinement method	Full matrix least-squares on F^2
Absorption correction	Semi-empirical from equivalents
Data/restraints/parameters	9589/120/955
Goodness-of-fit on F^2	1.05
Final R indexes [I>2σ (I)]	$R1 = 0.0756$, $wR2 = 0.1883$
Final R indexes [all data]	$R1 = 0.1215$, $wR2 = 0.2286$
Largest diff. Peak/hole (eÅ^{-3})	0.547 and -0.616

3. Results and Discussion

3.1. Synthesis and analysis of trans-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex

Trans-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex was made available in high yields *via* treating of $Cu(ClO_4)_2{\cdot}6H_2O$ with $4xMe_2N\text{-}Py$ ligand in alcoholic medium at RT condition as seen in Scheme 1. The *cis*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ possible isomer was not detected, possibly because to its lower stability caused by steric hindrance, resulting in considerable internal repulsion compared to the trans-isomer. Under RT stirred condition, the reaction processed smoothly since the mixture colour was changed from light blue to green bluish within one hour, resulting in the formation of the desired complex. In the solid state, the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex was found to has a high melting point, blue in colour, and stable in an O_2-open atmosphere. Furthermore, its structure was proved *via* SEM, CHN-EA, UV-Vis, TG/DTG, GC-MS, EDX, FT-IR, and XRD-crystal.



Scheme 1: Synthesis of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$.

The GCMS of the desired complex showed an excellent weak peak at m/z 751.2 (theoretical 752.4) supporting the formula weight of $[Cu^{II}(Me_2N\text{-}Py)_4(ClO_4)_2]^+$ complex, peak at m/z 652.2 can be attributed to one ClO_4 anion losing to form the mono-cation $[Cu^{II}(Me_2N\text{-}Py)_4ClO_4]^+$ stable fragment complex, losing of another ClO_4 to form the di-cation $[Cu^{II}(Me_2N\text{-}Py)_4]^{++}$ fragment complex can be cited to 552.2 m/z peak (Fig.1a). The atomic composition of the desired complex has been confirmed via EDX reflected the appearance of O, N, C, Cu and Cl atoms only indicating the purity of the crystal structure (Fig.1b). Moreover, the crystallinity and morphology were exterminated by SEM reflecting block particles as high crystalline rod-like morphology and complex purity (Fig.1c). Nevertheless, SEM reflected a high crystalline structure and free of any irregularity, agglomeration, defect, and high particle stability had been recorded (Fig.1c).

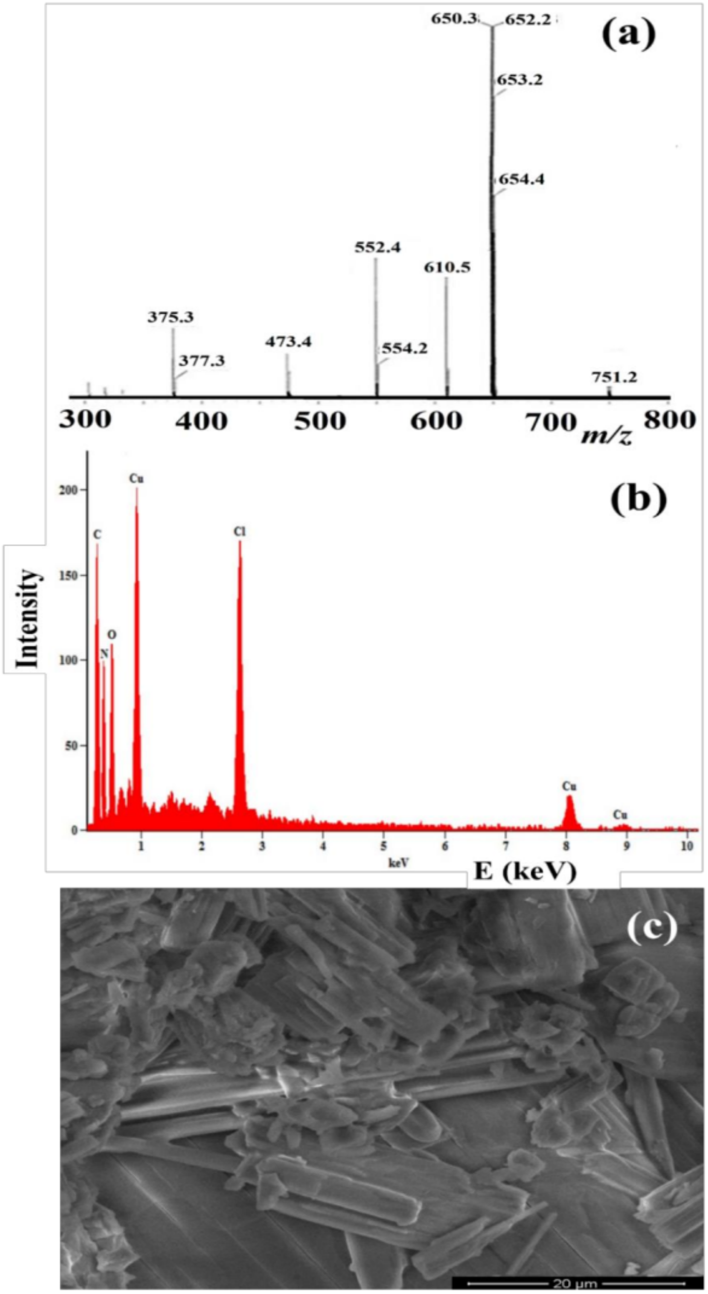


Fig.1. (a)GC-MS, (b)EDX, and (c)SEM of the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex.

In solid-state FT-IR (Fig.2a), the appearance of the stretching vibration strong band at 1092 cm^{-1} confirmed the existence of ClO_4 anion ligands in the complex backbone; moreover, the band at 3052 $\nu_{(Cph\text{-}H)}$, and 2960-2840 $\nu_{(CMe\text{-}H)}$ corresponded to Me_2N-Py ligands coordination. Additionally, peaks at 510-680 cm^{-1} $\nu_{(Cu-N)}/\nu_{(Cu-O)}$ supported the formation of Cu-N and Cu-O new bonds *via* L/M complexation process [27-30]. On the other hand, the UV-Vis behavior in MeOH reflected the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex with two absorption broadbands (Fig.2b), one in the UV area with λ_{max} = 277 nm ($\varepsilon = 1.2 \times 10^4$ $M^{-1}cm^{-1}$) attributed to π-to-π e-transition and band in the visible region with λ_{max} 698 nm ($\varepsilon = 8.2 \times 10^2$ $M^{-1}cm^{-1}$) attributed to d-to-d e-transition. The presence of such visible signal corresponded to the blue color of the solution, confirming the occurrence of N-centers of Me_2N-Py bonding to the Cu(II) center.

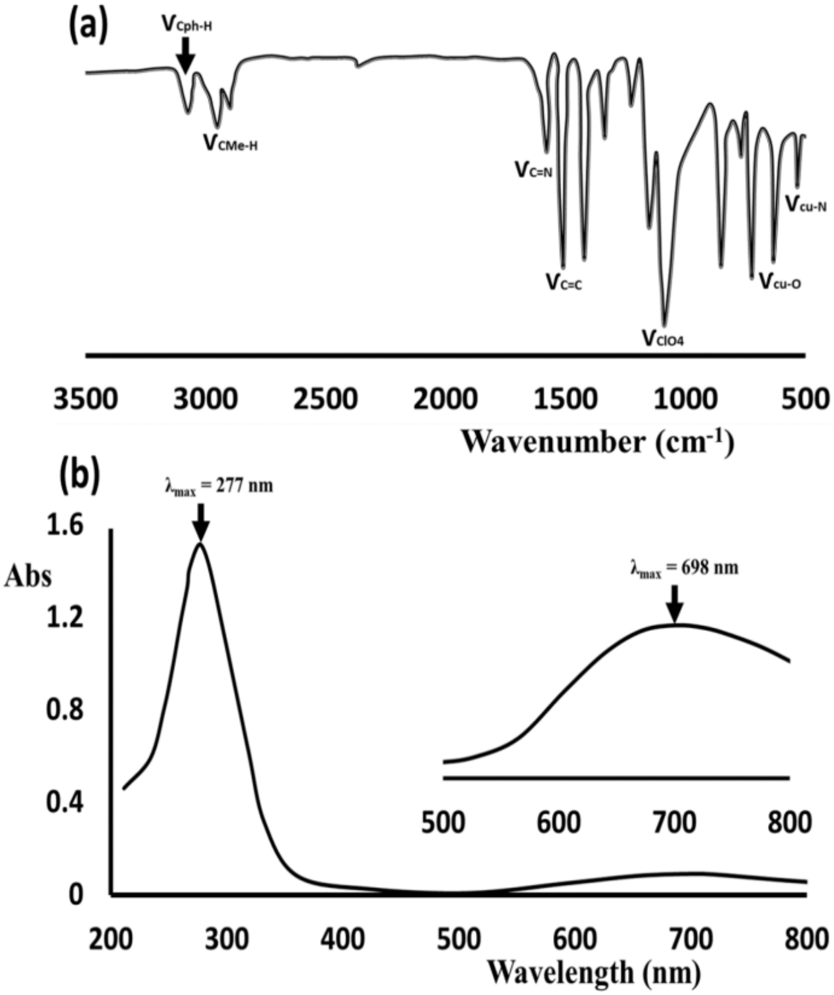


Fig.2. (a)Solid state FT-IR, and (b)UV-Vis of 1×10^{-4} M of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ dissolved in MeOH.

3.2. XRD of the trans-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)$ complex

The crystal and molecular structure of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ are depicted in Fig.3a and Table 2, which contains selective angles and bond lengths. The Cu(II) ion in the desired complex adopts an elongated octahedral (Oh) geometry [27-30], with six ligands coordinating it in a centrosymmetric manner (Fig.3b). This structure consists of four Me_2N-Py ligands with Cu-N bond lengths of Cu1-N1 = 2.000(6) Å, Cu1-N4 = 2.003(7) Å, Cu1-N5 = 1.994(6) Å, Cu1-N6 = 2.011(6) Å, Cu2-N10 = 2.011(6) Å, Cu2-N11 = 2.009(5) Å, Cu2-N12 = 2.664(11) Å and Cu2-N13 = 2.007(5) Å on the square planar. Additionally, there are two perchlorates positioned along the long z-axis, with a Cu-O bond length of Cu1-O1 = 2.676 (6) Å, Cu1-O15A = 2.73 (3) Å, Cu2-O14 = 2.733(6) Å and Cu2-O5B = 2.73(3) Å. The XRD analysis revealed that the Cu-O bond length around the Cu(II) central atom increased by 8% compared to similar systems [30, 31]. This provided evidence for the occurrence of the widely recognized elongation of the Jahn-Teller distortion. The elongation ratio between the average axial and equatorial bonds was found to be approximately 20%. Moreover, Oh indicated by the sum of the non-classical $C_{py}\text{-}H...O_{ClO3}$ and $C_{Me}\text{-}H...O_{ClO3}$ H-bond intermolecular forces within the 4 molecules existed in the unit cell as seen in Fig.3c. Moreover, H-bonds angles of the basal plane measuring 362.27° (Cu1/N3/N4/N5/N6) and 361.68° (Cu2/N1/N2/N13/N10) and the angle subtended by the atoms in the apical position for O1-Cu1-O15A and O14-Cu2-O5B is found to be 168.35° and 158.55°, respectively.

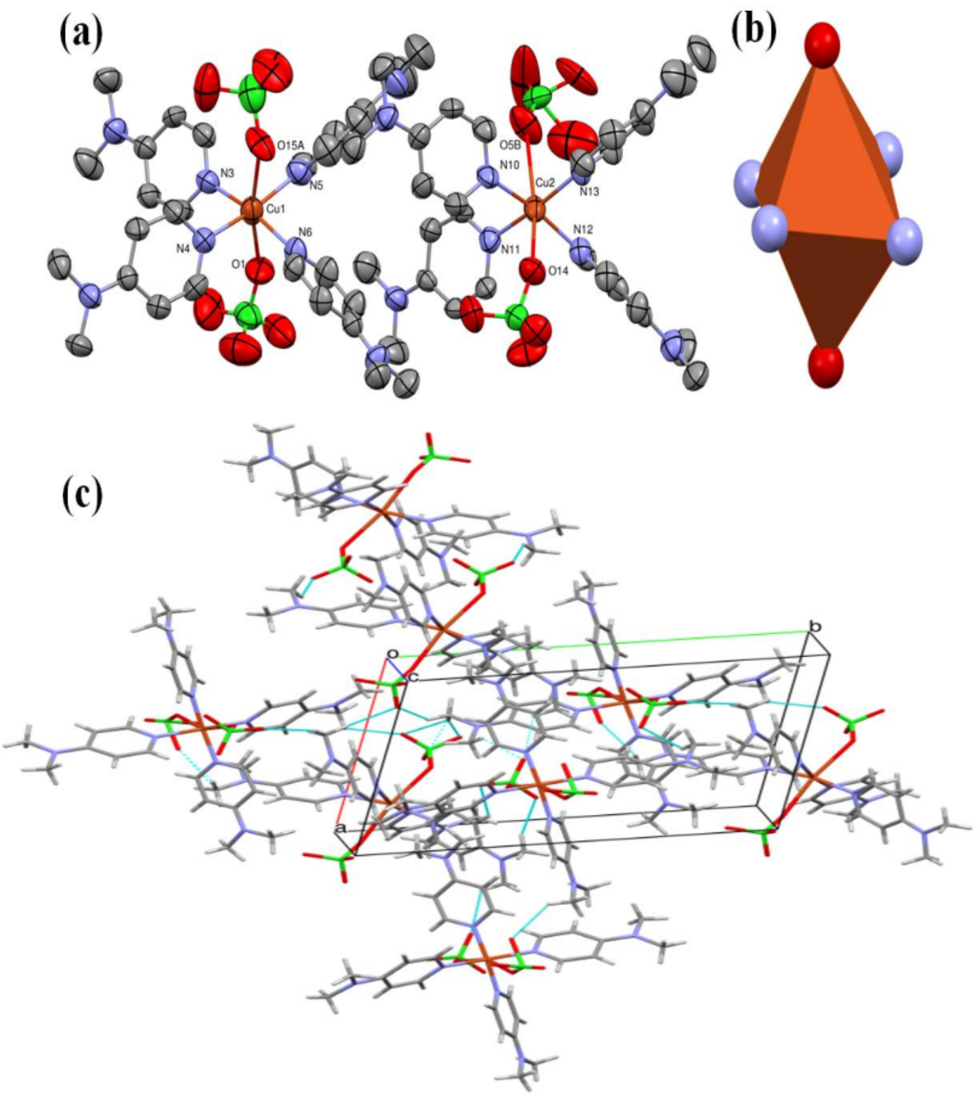


Fig. 3. (a)ORTEP, (b)elongation Jahn-Teller distortion, and (c)3D-molecular intermoleculars.

Table 2. Selected structure parameters of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$.

No.	Bond		Å	No.	Angle			(°)
1	Cu01	O007	2.737(6)	1	O007	Cu01	N008	87.2(2)
2	Cu01	N008	2.017(5)	2	O007	Cu01	N009	82.0(2)
3	Cu01	N009	2.012(5)	3	O007	Cu01	N00G	98.7(2)
4	Cu01	N00G	2.008(6)	4	O007	Cu01	N00I	91.0(2)
5	Cu01	N00I	2.015(6)	5	O007	Cu01	O2	176.5(3)
6	Cu01	O2	2.63(1)	6	N008	Cu01	N009	169.0(2)
7	Cl03	O007	1.429(6)	7	N008	Cu01	N00G	90.8(2)
8	Cl03	O00A	1.408(7)	8	N008	Cu01	N00I	89.2(2)
9	Cl03	O00P	1.413(7)	9	N008	Cu01	O2	90.2(3)
10	Cl03	O00R	1.411(6)	10	N009	Cu01	N00G	89.0(2)

11	N008	C00V	1.34(1)	11	N009	Cu01	N00I	92.8(2)
12	N008	C01L	1.324(8)	12	N009	Cu01	O2	100.7(3)
13	N009	C012	1.351(9)	13	N00G	Cu01	N00I	170.3(2)
14	N009	C01A	1.35(1)	14	N00G	Cu01	O2	83.6(3)
15	N00E	C00N	1.35(1)	15	N00I	Cu01	O2	86.7(3)

3.3. XRD/HSA-interactions investigation

The presence of ClO_4 anions as multi O contents plays a critical role in building several H-bonds interaction in the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex lattice as in Fig.4. The structural analysis revealed that the crystal packing is stabilized by the non-covalent interactions, especially the intermolecular non-classical H-bond interactions. The neighbouring molecules for the symmetry-independent molecule in the asymmetric unit are generated by non-classical C_{py}-H...O and C_{Me}-H...O intermolecular H-bonds (Table 3) resulting in the formation of 2 and 1D-dimensional supramolecular synthons molecular arrangement.

The crystal lattice of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ has two primary 2-D synthons. The S9 synthon was produced through non-classical C_{py}–H···$O_{perchlorate}$ and C_{Me}–H···$O_{perchlorate}$ hybrid hydrogen bonds, with bond lengths of 2.652 and 2.550 Å, respectively. In addition, another S6 synthon was formed by combining non-classical C_{Me}–H···$O_{perchlorate}$ and C_{py}–H···$O_{perchlorate}$ with distances of 2.731 and 2.899 Å, respectively (Fig.4b). In addition, the ClO_4 anions in *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ also engaged in interactions with adjacent complex molecules. For instance, one of the ClO_4 anions formed a non-classical pure 3C_{Me}–H···$O_{perchlorate}$ interactions, leading to the formation of 1D-intermolecular interactions all directions among the molecules, resulting an additional lattice stability, as depicted in Fig.4c.

Table 3. Total H-bond interactions per *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ molecule.

D-H...A	**D-H (Å)**	**H...A (Å)**	**D...A (Å)**	**D-H...A (°)**
C2-H2A...O2	0.96	2.55	3.473(12)	162
C2-H2B...O15	0.96	2.56	3.422(10)	149
C15-H15...O1	0.93	2.55	3.446(19)	161
C20-H20A...O13	0.96	2.55	3.420(12)	151
C36-H36A...O6	0.96	2.45	3.347(13)	155

C33-H36C...O2	0.96	2.53	3.271(12)	135
C15-H15...O1	0.93	2.56	3.056(11)	114
C5-H5...O5	0.93	2.28	3.037(17)	138
C12-H12...O7	0.93	2.55	3.446(19)	161
C34-H34...O13	0.93	2.54	3.313(10)	141
C47-H47...O14	0.93	2.55	3.156(10)	123
C50-H50...O12	0.93	2.48	3.105(13)	125

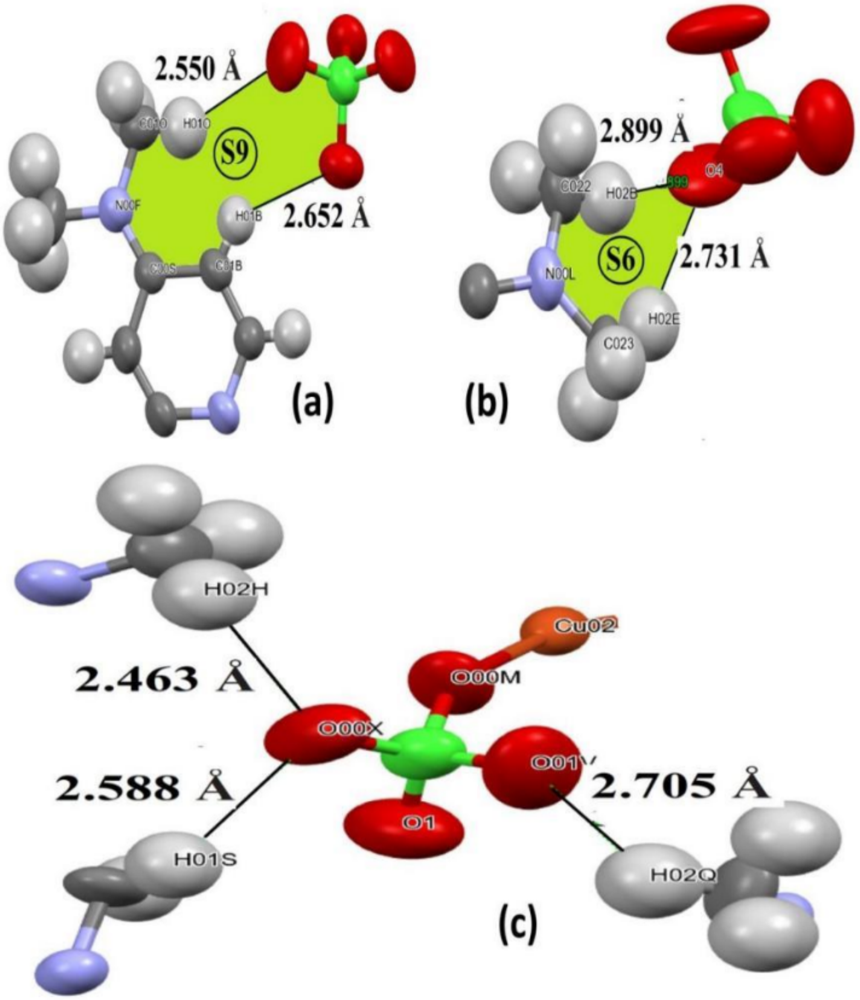


Fig.4. (a) 2D-S9, (b) 2D-S6 synthons, and (c) 1D-interactions around ClO_4 anion ligand.

The HSA is the most effective computational method for clarifying the intermolecular interactions in the XRD-resolved lattice of a certain complex structure [31-37]. The 3D-d_{norm} surfaces are graphed using a consistent color scale ranging from -0.3283 to 1.887 range. The examination of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ using HSA has verified the presence of multi-distinct red spots within the complex surface, the surface are with 14 spots as depicted in the d_{norm} surface (Fig.5a). Significantly, the greatest spots are located near the ClO_4 counterions, exhibiting non-classical C_{py}-H….O, and C_{Me}-H….O H-bond short interactions where no other h-bonds like H….N types have been recorded. In addition, the existence of electrophilic hydrogen atoms (blue) and nucleophilic terminal O (red) of the ClO_4 counterions (Fig.5b) on the molecule surface clarified the creation of these H-bonds. The high H….O contribution ratio of 17.5% compared to the low H….N ratio of 0.8% supported only the existence of C-H….O nonclassical H-bonds in the complex lattice, the other atom-to-atom (A-to-A) contribution ratios are illustrated in Fig.5c. The HSA-computational result agreed well with the experimental XRD one.

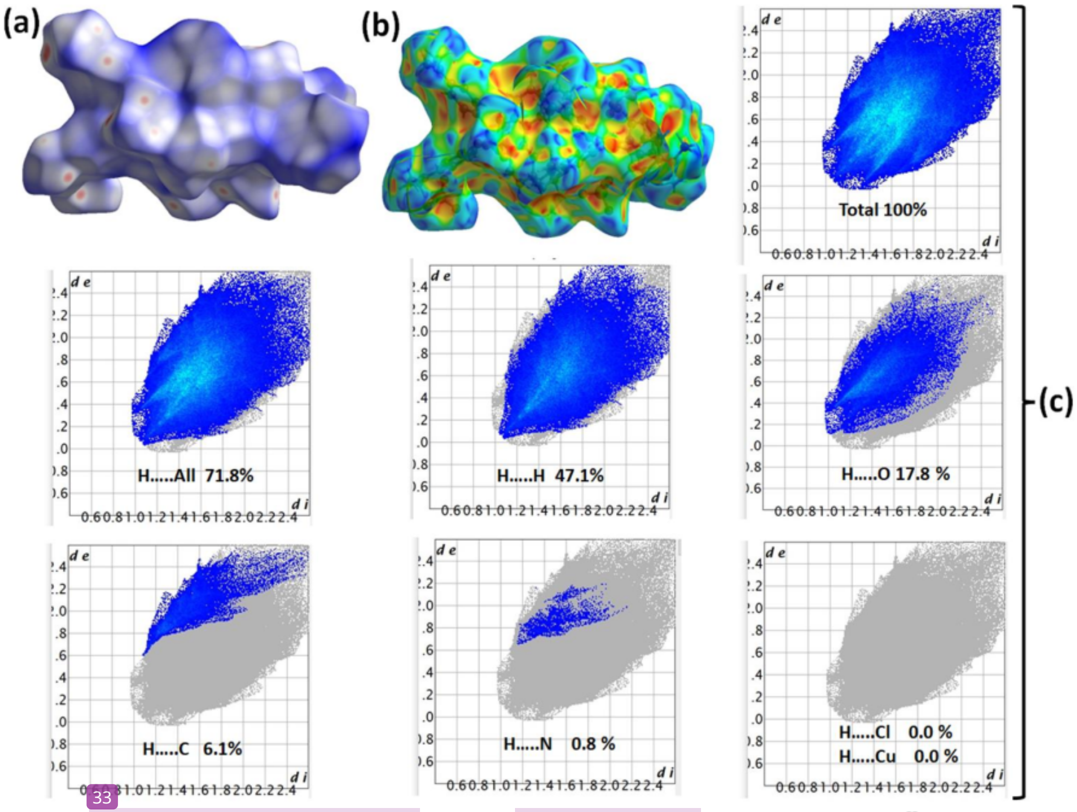


Fig. 5. (a) d_{norm}, (b) shape-index, and (c) A-to-A interactions ratios in *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$

3.4. TGA analysis

TG-DTG was performed to examine the thermal characteristics of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex (Fig.6). The TGA analysis showed that the complex undergoes a mass loss of 65.4% (Cal, 64.8%) in the temperature range of 210-395 °C and with T_{DTG} = 260 °C, this step was corresponding to the de-structured or decomposition of the Me_2N-Py organic ligands in the *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ to light gasses (CO_2 and NO_x) producing the nacked $Cu(ClO_4)_2$ complex. As the temperature increases, the $Cu(ClO_4)_2$ product experiences a further weight reduction of 23.2% (Cal, 22.9%) between temperatures of 580–710 °C and with T_{DTG} = 636 °C since ClO_4. The remaining residue corresponding to Cu=O final product (yielding 10.8%) was proved by FT-IR (Fig.2a).

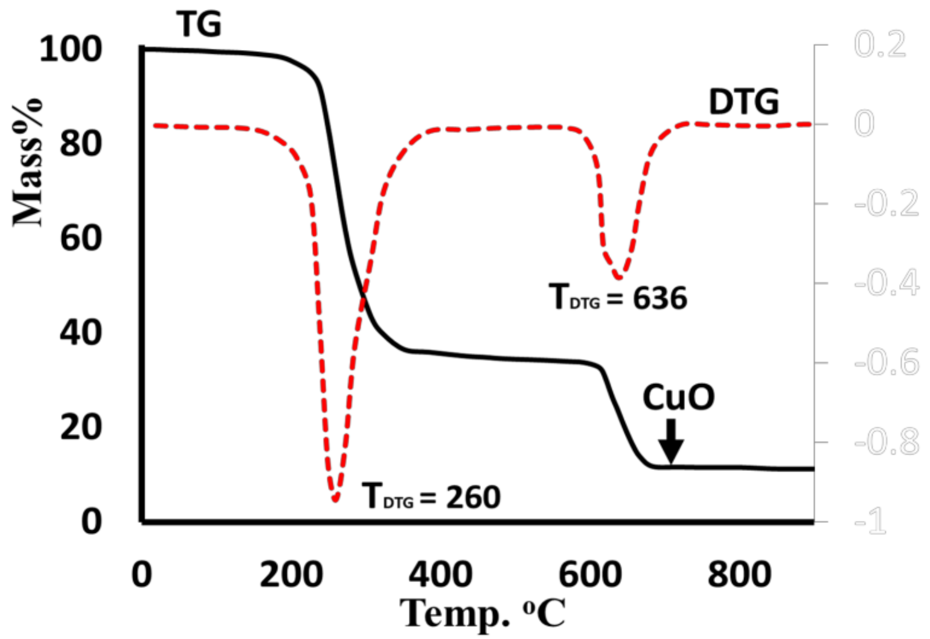


Fig.6. TG/DTG of *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex.

3.5. 1BNA DNA docking of trans-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$

Molecular docking was used to investigate the electrostatic, hydrophobic, and energetic interactions between *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ and DNA (PDB:1BNA), since the 1BNA is simple, short and free available. The desired complex occupied the major groove of the 1BNA DNA, and the intricate structure smoothly merged with complex structure volume (Fig.7a). Significantly, the complex showed binding behaviour similar to the cisplatin complex mode of interaction, as it bonded to both DNA helix through short three hydrogen bonding and one π-π interaction (Fig.7b). The protons of Pyridine ligands did not show any binding contributions, meanwhile, the protons of Me of dimethyl functional groups played the critical role in the formation of the non-classical H-bonds like DNA:A: DA6:OP2….H-CH_2N with 2.93 Å bond length and DNA:B: DT19:O4….H-CH_2N with 2.88 Å bond length (Fig.7c) reflecting a positive correlation between the number of formed H-bonds and the binding energy of the complex, which was observed to be -9.45 kcal/mol.

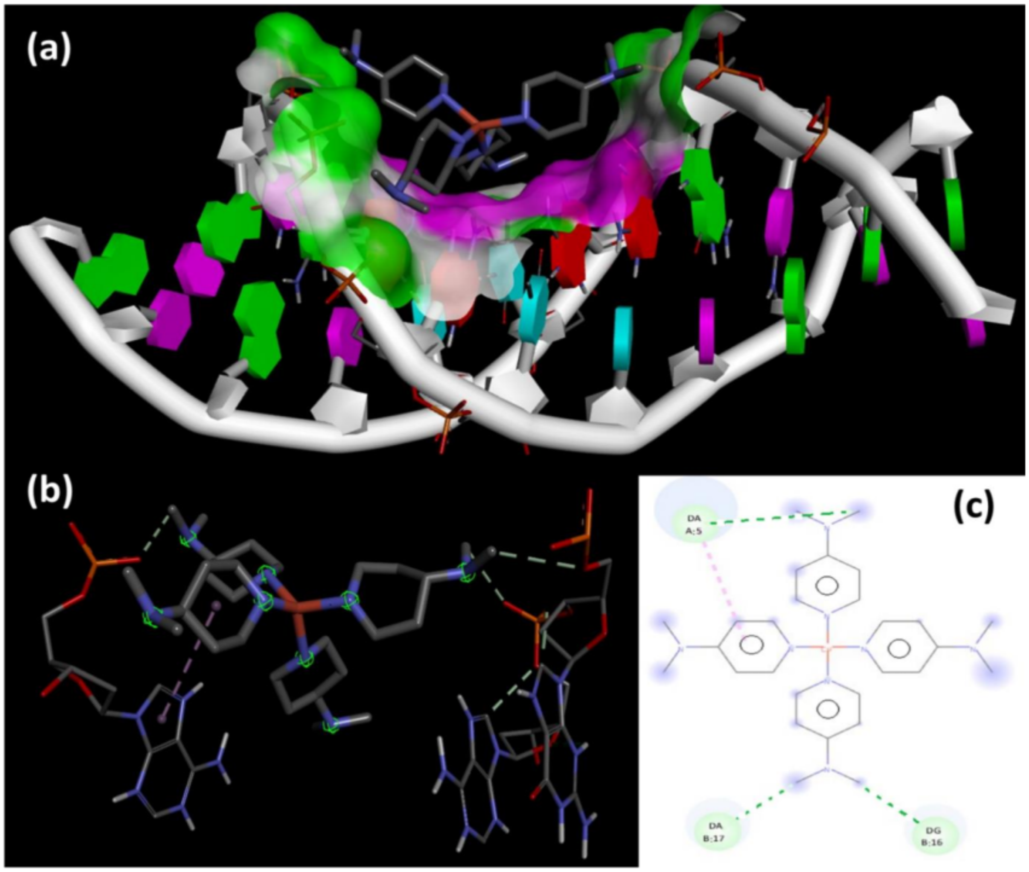


Fig.7. 1BNA DNA docking, (a) Major groove, (b) cisplatin mode, and (c) 2D-H-bonds interactions.

4. Conclusion

A novel *trans*-$(ClO_4)_2Cu^{II}(Me_2N\text{-}Py)_4$ complex was synthesized and investigated utilizing several physicochemical techniques in the current research study. The structural analysis determined that the desire complex exhibited crystalline properties in a triclinic crystal system with the P1 space group. The XRD of Cu(II) ion reflected a distorted Oh geometry, with two perchlorate ions positioned axially and four Me_2N-Py ligands organized in a planar shape. Additionally, XRD study has shown the presence of a dynamic Jahn-Teller elongation distortion, which has resulted in a 20% increase in the Cu-O bond lengths. The crystal packing is stabilized by various S9 and S6 synthons intermolecular hydrogen bonding constructed via C_{Me}-H...O and C_{ph}-H...O non-classical interactions. The TG/DTG represented the complex with high thermal stability and two steps degradation mechanism. Furthermore, the docking technique revealed the complex to be a good 1BNA major grove positional binder, showing 2 H-bonds and -9.45 kcal/mol binding energy.

5. Supplementary material:

The crystallographic data has been submitted to the Cambridge Crystallographic Data Centre and assigned the additional publication number CCDC **2287195.** To receive copies of this information, you can visit the website www.ccdc.cam.ac.uk/conts/ retrieving.html. Alternatively, you can contact the CCDC at their physical address: 12 Union Road, Cambridge CB2 1EZ, UK. You can also send a fax to +44-1223-336033 or an email to deposit@ccdc.cam.ac.uk. There is no charge for obtaining these copies.

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