



Synthesis, crystal structure, antibacterial activity and theoretical studies on a novel Zn(II) complex based on 2,4,6-tris(2-pyridyl)-1,3,5-triazine ligand

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ABSTRACT

It is known that 2,4,6-tris(2-pyridyl)-1,3,5-triazine (tptz) also belongs to noticeable building blocks in both organic and inorganic supramolecular chemistry. We have prepared new Zn(II) complex of 2,4,6-tris(2-pyridyl)-1,3,5-triazine. The new metal complex was characterized by elemental analysis, IR spectra, UV spectra measurements. The molecular structure of $[Zn(tptz)(Cl)_2]$ was investigated by X-Ray single crystal technique. From all data, the stoichiometry of the complex was found to be 1:1 (metal/ligand). The all data indicated that the tptz exhibits major coordination site behavior. Potential energy surface (PES) was calculated using the DFT / B3LYP / 6-311 G (d, p) method to determine the lowest energy state of the molecular structure. Geometric structure parameters and vibration wavenumbers calculated according to the lowest energy state were compared with experimental data. The electronic properties such as frontier molecular orbital analysis and Uv-Vis spectrum obtained at acetonitrile solvent and gas phase were also studied. The $[Zn(tptz)(Cl)_2]$ complex was screened for antibacterial activity against Gram-positive, Gram-negative and yeast by using minimal inhibitory concentration method (MIC). $[Zn(tptz)(Cl)_2]$ has been found to show significant antimicrobial effects on gram (-), gram (+) and eukaryotic yeast. The DNA binding interactions was also determined experimentally by spectrophotometric and electrochemical methods.

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1. Introduction

Multidentate ligands containing two or more pyridine donor units are known as polypyridyl ligands [1]. Polypyridyl derivatives are widely used as ligands in coordination chemistry and as building blocks for the generation of supramolecular structures. Among the polypyridyl ligands, tptz has drawn much attention for its multiple coordination sites (major, middle, and minor) and the large stabilizing π systems (Scheme 1) [2–4].

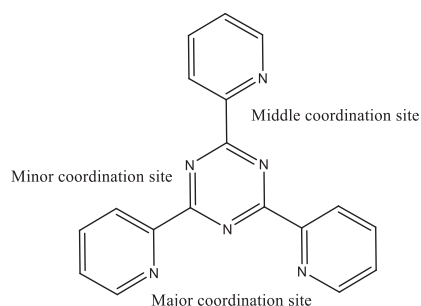
Having three 2-pyridyl rings fixed on a central 1,3,5-triazine platform, 2,4,6-tris(2-pyridyl)-1,3,5-triazine (tptz) also belongs to noticeable building blocks in both organic and inorganic supramolecular chemistry. It attracts scientific interest due to non-

covalent π - π stacking ability, directional hydrogen bonding and coordination properties [5]. Therefore, the tptz ligand has different coordination modes.

The planar structure of tptz along with its large π system also makes it a suitable candidate for further chemical modifications. tptz has potential in pharmacologically active coordination compounds and has been shown to be a useful ligand in coordination chemistry [6]. Derivatives of 1,3,5-triazine have received much attention as they have shown promising potential as antitumor agents, enzyme inhibitors and other forms of bioactivity [7–9]. tptz derivatives are used in the synthesis of new materials, as analytical reagents, preparation of DNA cleaving agents and in the design of supramolecular complexes [3,10–12]. In addition, transition metal complexes of tptz also have gained much attention because of their biological activity and their physical, magnetic, and photoluminescence properties [12–15].

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Scheme 1. The three coordination sites in tptz.

In this work, Zn(II) complexes of 2,4,6-tris(2-pyridyl)-1,3,5-triazine ligand have been synthesized. The resulting complex was characterized by elemental analyses, IR and UV-Vis. spectral studies. The structure of $[Zn(tptz)(Cl)_2]$ complex has been investigated by using X-Ray Single Crystal method. All compounds were examined for antimicrobial activity against pathogenic strains (*Gram-negative and Gram-positive bacteria*).

2. Experimental

2.1. Materials

All chemicals which used in this research was purchased from Sigma/Aldrich. All chemicals purchased from commercial suppliers were of reagent grade and were used without further purification.

2.2. Physical measurements and computational details

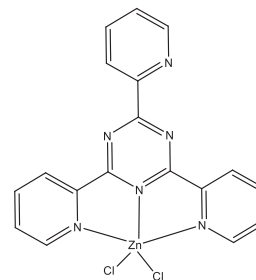
The elemental analysis were recorded on Thermo Flash 2000 Elemental Analyser. The electronic absorption spectra of title compound were recorded at room temperature in acetonitrile solution on a Thermo Evolution UV-Visible Spectrophotometers working between 200 and 800 nm. IR spectrum was recorded on Thermo Scientific Nicolet iS10 FT-IR spectrophotometer using ATR. The structural properties of $[Zn(tptz)]$ molecule, DFT / B3LYP method and 6/311-G (d, p) base set were used for spectroscopic and electronic structure analysis [16–18]. The potential energy surface (PES) calculated without force symmetry was examined and the most stable structure was determined. Vibration analysis is the most stable structure optimized and vibration assignments are made with Veda4 program [19]. UV-Vis and boundary molecule orbitals were examined by B3LYP method to determine the electronic structure [20]. GAUSSIAN 09 program package was used on the basis of calculations [21].

2.3. X-Ray crystallography

X-ray crystallography was performed at 293 K on a Bruker D8 QUEST diffractometer (BRUKER APEX-II CCD) employing graphite-monochromated Mo-K α radiation. The structure was solved by intrinsic phasing method and refined by full-matrix least-squares methods with anisotropic thermal parameters for all non-hydrogen atoms. The hydrogen atoms were inserted at their calculated positions, and fixed there. All calculations were carried out on a Windows 7 Core i7 computer using SHELXT 2014/5 and SHELXL-2016/4 [22,23]. Crystallographic data have been deposited with Cambridge Crystallographic Data center (Deposit numbers CCDC 1841037). Crystal data and details related to the data collection are given in Table 1.

Table 1
Crystal Data and experimental data of $[Zn(tptz)(Cl)_2]$.

Chemical formula: $C_{18}H_{12}N_6Cl_2Zn$	
Formula weight = 448.61	
$T = 293$ °K	
Crystal system: Monoclinic	Space group: P 21/n
$a = 12.7662(11)$ Å	$B = 99.150(3)$ °
$b = 10.6276(9)$ Å	$Z = 4$
$c = 13.8146(12)$ Å	
$V = 1850.4(3)$ Å ³	
Radiation Mo K α ($\lambda = 0.71073$ Å)	
μ (Mo K α) = 1.632 mm ⁻¹	$F(000) = 904$
Crystal Size = 0.02 × 0.03 × 0.04 mm ³	
No. of reflections collected = 29,835	
No. of independent reflections = 3782	
θ range for data collection: 2.99° to 26.40°	
Data/Restraints/Parameters = 3782/0/244	
Goodness-of-fit on $F^2 = 1.040$	
R indices [$I > 2\sigma(I)$]: $R1 = 0.0733$, $wR2 = 0.1506$	
R indices (all data): $R1 = 0.1059$, $wR2 = 0.1634$	
$(\Delta\rho)_{max} = 0.435$ e Å ⁻³ ($\Delta\rho)_{min} = -0.433$ e Å ⁻³	
Measurement: Bruker APEX-II CCD	
Programs system: Bruker SAINT	
Structure refinement: SHELXT 2014/5	
Structure determination: SHELXL-2016/4	
CCDC deposition number: 1,841,037	



Scheme 2. Synthesis of $[Zn(tptz)(Cl)_2]$.

2.4. Preparations

2.4.1. Synthesis of $[Zn(tptz)(Cl)_2]$

A solution of $ZnCl_2$ (0.136 g, 1 mmol) in methanol (10 mL) was added to a hot solution containing 2,4,6-tris(2-pyridyl)-1,3,5-triazine (0.312 g, 1 mmol) in methanol (20 mL). The reaction mixture was refluxed for 3–4 h. and then left the cool. gray color crystals were obtained in 2 days. Yield: 58%, Mp(decomp.): 280 °C. Elemental Anal. Found (Calcd.) (%): C: 47.98 (48.19), H: 2.65 (2.70), N: 18.65 (18.73). The chemical structure of 1 is shown in Scheme 2.

2.4.2. Detection of antibacterial activity

Standard bacteria were used for antimicrobial activity study. In this study conducted according to the minima linhibitory concentration (MIC) method, Gram positive (*Staphylococcus aureus* ATCC 6538P, *Bacillus cereus* ATCC 10,876), Gram negative (*Escherichia coli* ATCC 25,922, *Pseudomonas aeruginosa* ATCC 27,853) and yeasts (*Candida albicans* ATCC 10,231). The stock solution of the newly synthesized compound used in this study was prepared by dissolving in DMSO. All microorganism cultures were prepared by incubating in suitable media for 24 h at 37 °C. Microorganisms were grown in 50 ml nutrient broth for 24 h. The density of the bacteria obtained after 24 h was prepared as 10⁶ bacteria per milliliter. At the same time, this value is accepted in accordance with 0.5 McFarland standards. After adding 1 ml of the obtained bacterial solution to the tubes, serial concentration is added by adding a suitable concentration of substance. All samples are incubated at 37 °C for 24 h incubation. The last tube without growth is recorded as a MIC value (μ g/ml).

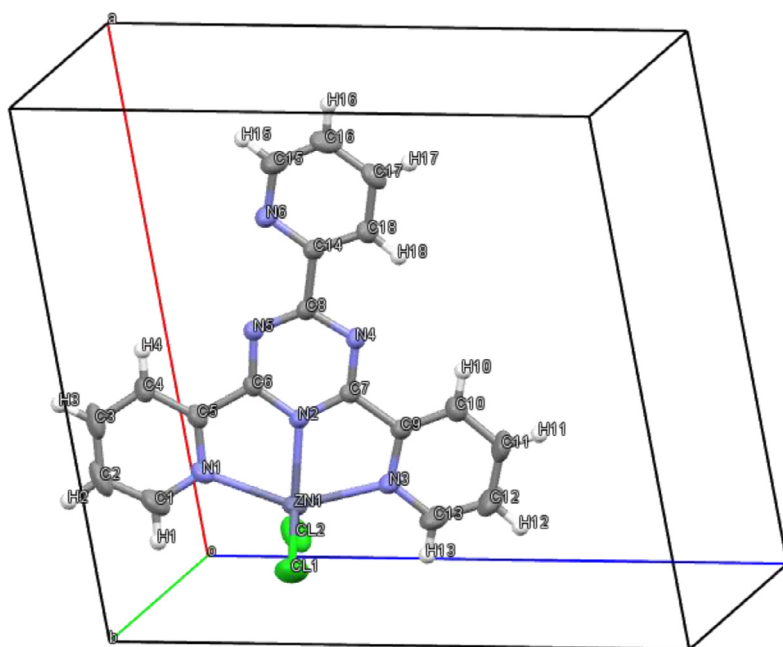


Fig. 1. The molecular structure of $[Zn(tptz)(Cl)_2]$.

2.4.3. DNA interaction studies

pBR322 plasmid DNA hydrolytic cleavage activity of $[Zn(tptz)(Cl)_2]$ has been determined by agarose gel electrophoresis. Compound treated with 0.25 ppm *pBR322* plasmid DNA. Final concentration of compound was between 1 and 3 mM. Nontreated and DMSO treated *pBR322* DNA were used as control. H_2O_2 was used as activator. The DNA interaction reaction was carried out at 37 C for 3 h. After incubation period 1 μ l 6X gel loading buffer was added samples then loaded on 1% agarose gel for 90 min at 80 V in TBE buffer (pH 8). Gels were stained with ethidium bromide for 15 min and were washed deionized water for 15 min. Then gels were photographed under UV light.

3. Results and discussion

3.1. Structure description of $[Zn(tptz)(Cl)_2]$

The structure of $[Zn(tptz)(Cl)_2]$ was determined by X-Ray crystallography. The molecular structure obtained from X-ray analysis results are shown in Fig. 1. The selected bond lengths and angles are summarized in Table 2. The crystal packing is governed by intramolecular C–H...Cl hydrogen bonds. In the structure of complex species (Fig. 1), a single Zn(II) metal center binds to the tptz ligand in a tridentate fashion through a single N atom from the central triazine ring and N atoms from two of the three pyridyl rings. Two

chloride ions complete the coordination of the Zn(II) cation. An ORTEP view of compound is shown in Fig. 2. The Zn atom is linked to two Cl and three N atoms to form a trigonal bi-pyramidal environment where the Zn–N bond lengths range from 2.081(4) Å – 2.279(5) Å and Zn–Cl bond lengths are 2.2258(18) Å – 2.2502(18) Å. The angle values of trigonal bi-pyramidal environment, centered with Zn atom, range from 73.00(16)^o (N2–Zn1–N1) and 146.51(16)^o (N1–Zn1–N3) (Table 2). The coordination planes and their intersects angles has been calculated and listed in Table 3. The stabilization of the crystal structure arises from electrostatic interactions and is assisted by intermolecular C–H...Cl hydrogen bonds with C...Cl distances are 3.764 Å; 3.508 Å and 3.761 Å respectively between the layers (Table 4) Fig. 3.

3.2. IR studies of $[Zn(tptz)(Cl)_2]$

In the FT-IR spectrum of free tptz, the three bands were observed at 1524, 1468 and 1434 cm^{-1} cm due to the pyridyl ring ($\nu_{C=N}$, $\nu_{C=C}$) [3]. In the spectrum of $[Zn(tptz)(Cl)_2]$ complex, these values shifted and were observed at 1556, 1531 and 1473 cm^{-1} , respectively. The intense band of the tptz spectrum at 1369 cm^{-1} cm is assigned to the stretching vibrations of central triazine ring. After the formation of the complexes, this peak was observed at 1374 cm^{-1} , indicating that center ring nitrogen atom coordinated to the metal ion. The peak at 999 cm^{-1} is attributed to bending vibration of pyridyl ring and in the IR spectra of $[Zn(tptz)(Cl)_2]$ complex, it was observed 1008 cm^{-1} [3,24,25]. In summary, in the complex, tptz coordinated to metal ion by the three nitrogen atoms of the major coordination sites Fig. 4.

3.3. UV–Vis. studies of $[Zn(tptz)(Cl)_2]$

From previous studies, it is known that the absorption band of the ligand is observed at 278 nm [26]. After formation of the complex, a red shift of 11 nm was observed in this band. These change indicated that tptz coordinated with the metal ion in the complex Fig. 5.

Table 2
Selected geometric parameters, bond lengths and angles (Å, °).

Bond	Bond length (Å)	Bond	Bond angle (°)
Zn1 - N2	2.081(4)	N2-Zn1-Cl2	120.20(14)
Zn1 - Cl2	2.2258(18)	N2-Zn1-Cl1	119.27(14)
Zn1 - Cl1	2.2502(18)	Cl2-Zn1-Cl1	120.48(8)
Zn1 - N1	2.271(5)	N2-Zn1-N1	73.00(16)
Zn1 - N3	2.279(5)	Cl2-Zn1-N1	99.83(14)
N2 - C6	1.336(7)	Cl1-Zn1-N1	99.05(14)
N2 - C7	1.337(7)	N2-Zn1-N3	73.64(16)
		Cl2-Zn1-N3	94.34(13)
		Cl1-Zn1-N3	99.56(14)
		N1-Zn1-N3	146.51(16)

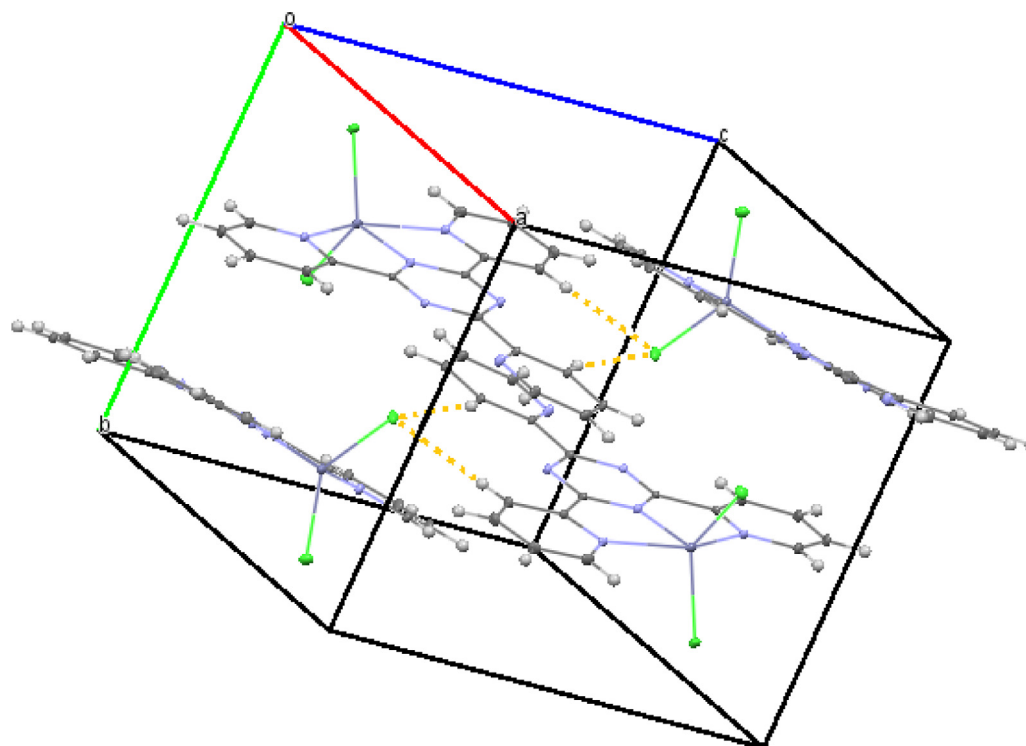


Fig. 2. Intermolecular Hydrogen Bonds in the Structure $[Zn(tptz)(Cl)_2]$.

Table 3

The coordination planes and their intersects angles.

Plane	Atoms	Rms deviation of fitted atoms	Description
Plane - 1	C14-C15-C16-C17-C18-N6	0.0024	Coplanar
Plane - 2	C1-C2-C3-C4-C5-C8-C9-C10-C11-C12-C13-Zn1-N1-N2-N3-N4-N5	0.0468	Nearly Coplanar
Plane - 3	Zn1-Cl1-Cl2	0.0000	Perfect Coplanar
Plane - 4	Zn1-N1-N2-N3	0.0269	Nearly Coplanar
Plane - A	Plane - B	Angle ($^\circ$)	
Plane - 1	Plane - 2	11.673 (0.088)	
Plane - 2	Plane - 3	89.655 (0.051)	
Plane - 3	Plane - 4	88.251 (0.102)	

Table 4

Inter-molecular hydrogen bonds geometry (\AA , $^\circ$).

D-H... A	d(D-H) (\AA)	d(H... A) (\AA)	D-H... A ($^\circ$)	d(D...A) (\AA)
C18-H18- Cl2 ⁽ⁱ⁾	0.930	2.898	155.43	3.764
C10-H10- Cl2 ⁽ⁱ⁾	0.930	2.642	155.27	3.508
C15-H15-Cl1 ⁽ⁱⁱ⁾	0.930	2.967	144.29	3.761

Symmetry codes: (i): $[x + 1/2, -y + 1/2, z + 1/2]$; (ii): $[x + 1, y, z]$.

3.4. Antimicrobial activity of $[Zn(tptz)(Cl)_2]$

The effect of $[Zn(tptz)(Cl)_2]$ on microorganisms was determined according to the MIC method. In this study based on serial dilution, MIC value for DMSO used as a control was found to be $>4000 \mu\text{g/ml}$. In contrast, $[Zn(tptz)(Cl)_2]$ has been found to show significant antimicrobial effects on gram (-), gram (+) and eukaryotic yeast. As a matter of fact, when the effect of $[Zn(tptz)(Cl)_2]$ on gram (-) bacteria is examined, it is seen that MIC values are $125 \mu\text{g/ml}$ for *E.coli* and $62.5 \mu\text{g/ml}$ for *Paeruginosa*. In addition, when looking at antimicrobial effect values (MIC) for gram (+), it was found to be $125 \mu\text{g/ml}$ for *S. aureus* and $500 \mu\text{g/ml}$ for *B.cereus*. To study the effect of $[Zn(tptz)(Cl)_2]$ on eukaryotes, yeast *C.albicans* was used. When the MIC value of *C.albicans* is investigated, it can be seen in the Table 5 where it is $250 \mu\text{g/ml}$.

3.5. pBR322 plasmid DNA hydrolytic cleavage activity

DNA Cleavage activity of compound was evaluated by conversion of pBR322 DNA supercoiled form to nicked circular and linear form. 50 mM Tris-HCl (pH: 8) (Lane 1) and DMSO (Lane 2) were used as control groups. The results of the agarose gel electrophoresis were shown in Fig. 6.

Complex didn't show any nuclease activity on pBR322 plasmid DNA absence of H_2O_2 . The percentage of nicked circular form increased in complex terated pBR322 DNA in the presence of H_2O_2 . Complex showed dose dependent nuclease activity by cutting DNA from a single strand in the presence H_2O_2 .

- a) Lane 1: pBR322 DNA control in 50 mM Tris-HCl buffer (pH: 7,2)
 Lane 2: pBR322 DNA + DMSO control
 Lane 3: pBR322 DNA + 3 mM complex
 Lane 4: pBR322 DNA + 2 mM complex
 Lane 5: pBR322 DNA + 1 mM complex
 b) Lane 1: pBR322 DNA control in 50 mM Tris-HCl buffer (pH: 7,2) + 30 mM H_2O_2
 Lane 2: pBR322 DNA+DMSO+ 30 mM H_2O_2
 Lane 3: pBR322 DNA + 3 mM complex+ 30 mM H_2O_2
 Lane 4: pBR322 DNA + 2 mM complex+ 30 mM H_2O_2
 Lane 5: pBR322 DNA + 1 mM complex+ 30 mM H_2O_2

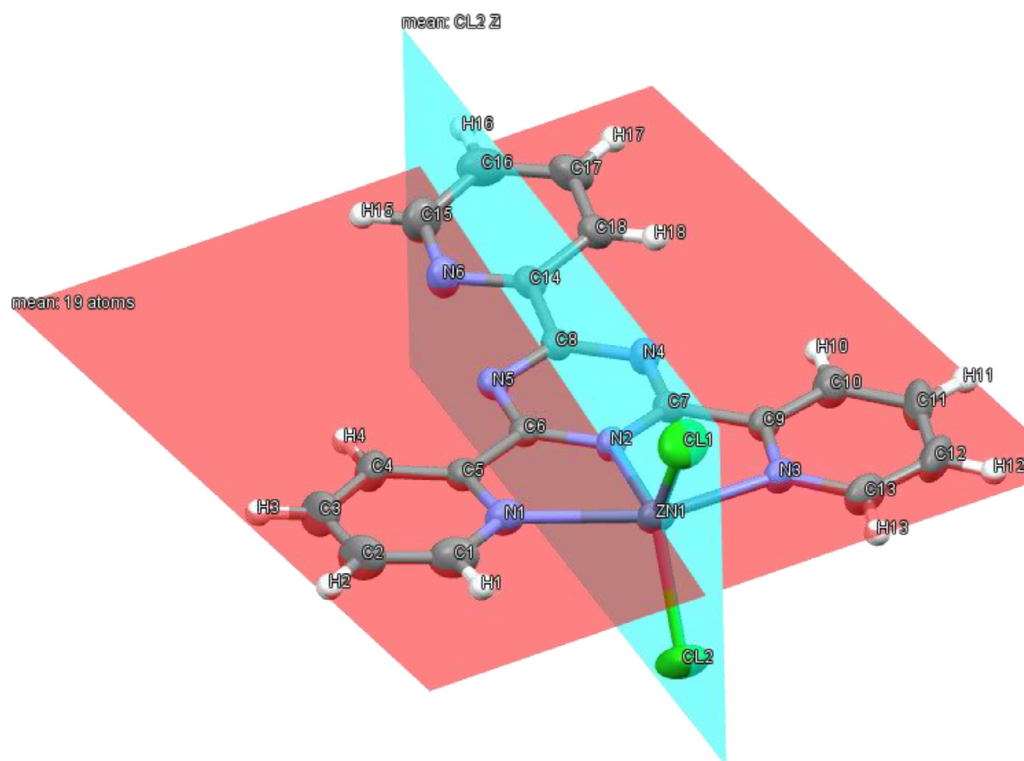


Fig. 3. View of the planes of $[\text{Zn}(\text{tpzt})(\text{Cl})_2]$.

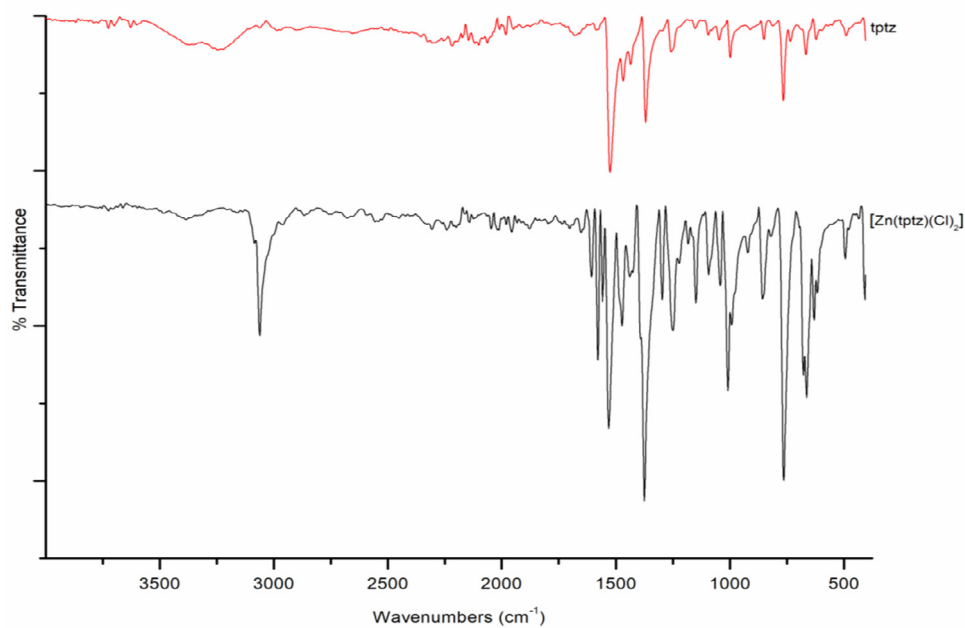


Fig. 4. IR spectra of the tpzt and $[\text{Zn}(\text{tpzt})(\text{Cl})_2]$.

Table 5

Minimal inhibitory concentration (MIC) values of the complex against on microorganisms ($\mu\text{g mL}^{-1}$).

	Gram Negative Bacteria ($\mu\text{g/ml}$)		Gram Positive Bacteria ($\mu\text{g/ml}$)	Yeast ($\mu\text{g/ml}$)	
	<i>E. coli</i> ATCC 25,922	<i>Pseudomonas aeruginosa</i> ATCC 27,853	<i>Bacillus cereus</i> ATCC 10,876	<i>Staphylococcus aureus</i> ATCC 6538P	<i>Candida albicans</i> ATCC 10,231
$[\text{Zn}(\text{tpzt})(\text{Cl})_2]$	125	62.5	500	125	250
DMSO	>4000	>4000	>4000	>4000	>4000

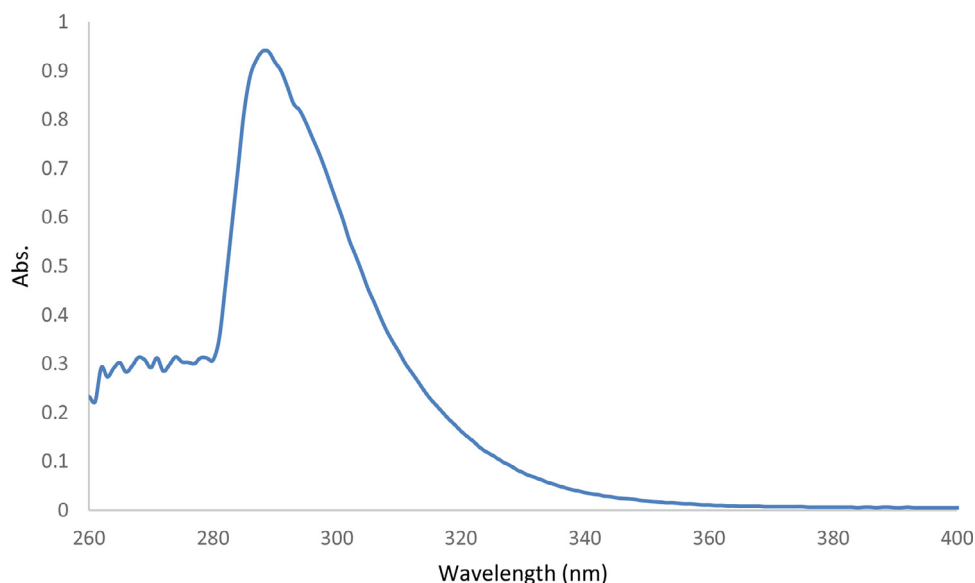


Fig. 5. Absorption spectra of $[Zn(tptz)(Cl)_2]$ (10^{-5} M).

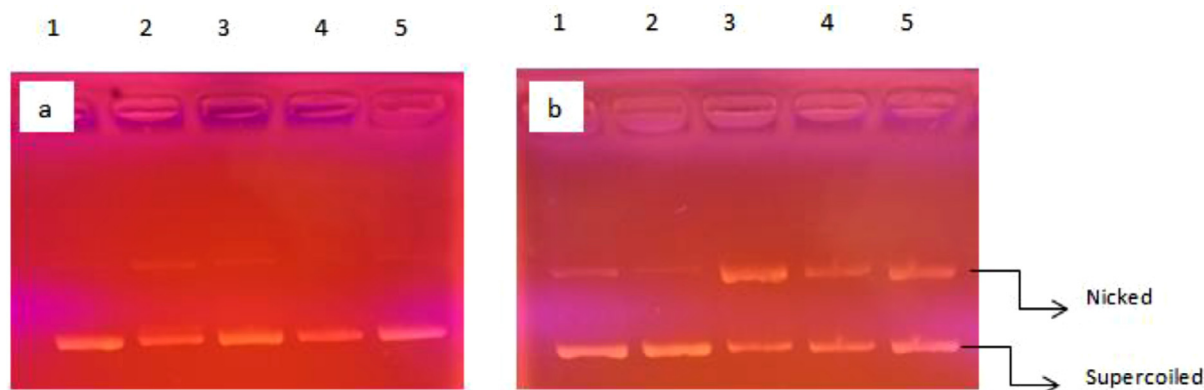


Fig. 6. Cleavage of pBR322 plasmid DNA by complex without H_2O_2 (a) and with H_2O_2 (b).

3.6. Computational studies of $[Zn(tptz)(Cl)_2]$

3.6.1. Potential energy surface (PES) and structural analysis

The potential energy surface is usually calculated from single bonds, which are thought to change the energy of the molecule. There is one single carbon bond (C8-C14) in the $[Zn(tptz)(Cl)_2]$ complex. The phenyl ring connected to the single carbon bond in the structure was changed by 10° in the range of $0-360^\circ$ and its energy was calculated in 36 steps. The torsional angle calculated for the molecule is N5-C8-C14-N6 and the Potential Energy Surface (PES) is shown in Fig. 7. By analyzing this graph, the molecular geometry of the $[Zn(tptz)(Cl)_2]$ complex was optimized using the B3LYP / 6-311 G (d, p) level for the lowest energy state. The lowest vibration frequency was determined as positive without any symmetry force.

The optimized geometric parameters of the molecule are given in Table 6. The global minimum energy of the molecule on the basis of optimized structure was -3721.821 Hartree. Zn-N bond lengths in the title molecule were calculated as 2.12, 2.30 and 2.29 Å and Zn-Cl bond lengths were calculated as 2.26 Å. The C-C bond lengths in the $[Zn(tptz)]$ molecule were generally calculated as 1.39 Å and the C-N bond lengths as 1.33 and 1.34 Å. The bonds formed by bonding hydrogen-bond carbon atoms to the nitrogen atom are usually 1.33 Å.

Table 6

The selected some bond parameters of the $[Zn(tptz)(Cl)_2]$.

Bond	Bond length (Å)		Bond	Bond angle ($^\circ$)	
	EXP.	B3LYP		EXP.	B3LYP
Zn1 - N2	2.081(4)	2.1199	N2-Zn1-Cl2	120.20(14)	117.4440
Zn1 - Cl2	2.2258(18)	2.2577	N2-Zn1-Cl1	119.27(14)	113.4019
Zn1 - Cl1	2.2502(18)	2.2610	Cl2-Zn1-Cl1	120.48(8)	1,291,407
Zn1 - N1	2.271(5)	2.2902	N2-Zn1-N1	73.00(16)	72.8993
Zn1 - N3	2.279(5)	2.3018	Cl2-Zn1-N1	99.83(14)	97.8144
N2 - C6	1.336(7)	1.3366	Cl1-Zn1-N1	99.05(14)	97.7492
N2 - C7	1.337(7)	1.3357	N2-Zn1-N3	73.64(16)	72.3770
			Cl2-Zn1-N3	94.34(13)	96.9493
			Cl1-Zn1-N3	99.56(14)	96.9482
			N1-Zn1-N3	146.51(16)	145.2553

3.6.2. Vibrational analysis

The vibration spectrum of the $[Zn(tptz)(Cl)_2]$ complex molecule was calculated by the B3LYP/6-311G(d,p) method, and the wavenumbers found were fit with the scaling factor 0.967. Vibration assignments were made with the VEDA4 program. The $[Zn(tptz)(Cl)_2]$ molecule has 111 basic vibration modes. 12 of these bands are pure bands and are assigned as C-H stretching bands. C-H stretching bands are in the range of $3118-3049\text{ cm}^{-1}$. This band is also seen in the experimental IR spectrum. The sharpest

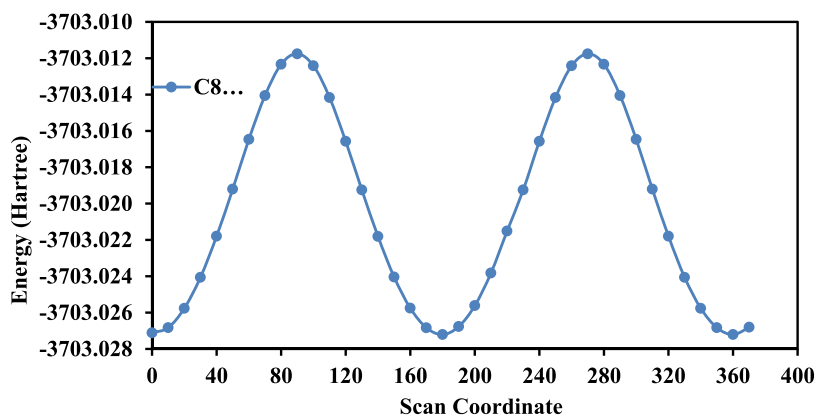


Fig. 7. Potential Energy Surface (PES) of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$.

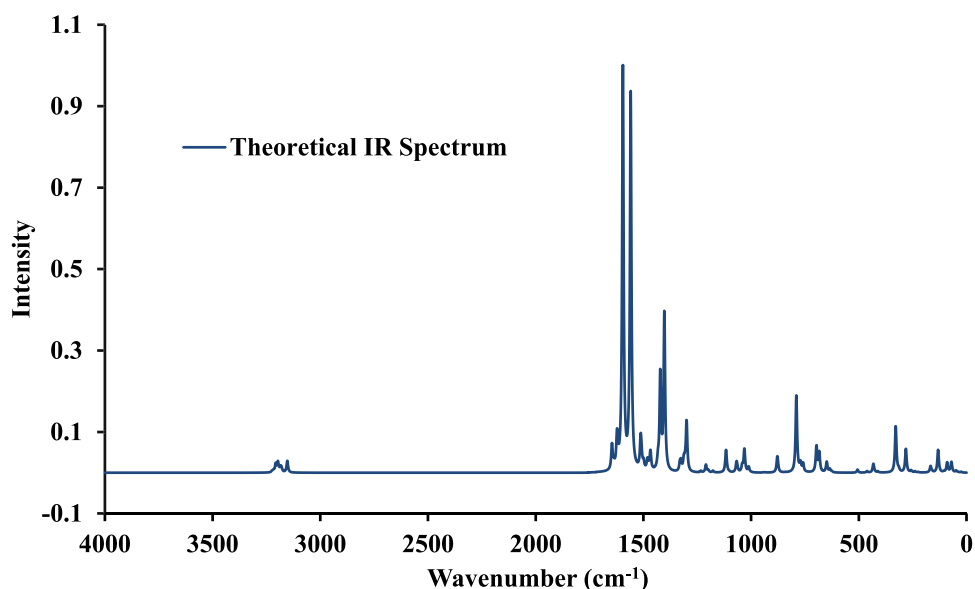


Fig. 8. Theoretical IR spectrum of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$.

peaks in the molecule are seen at 1543 and 1507 cm^{-1} it is seen in Fig. 8. These bands are assigned as the stretching vibration of the C=N and C=C double bonds. The Zn-Cl bond stretching vibration of the $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ complex molecule was calculated at 272 and 318 cm^{-1} .

3.6.3. Frontier molecular orbitals analysis

The conductivity band is called LUMO, the lowest unoccupied molecular orbital, and the valence band is HOMO, the highest occupied molecular orbital. The transition between these orbitals is concentrated among the atom groups and gives important information about the transfer of molecules within the molecule [27]. To determine the charge transfer in the molecule, the most important transition of the $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ molecule is drawn in Fig. 9. The HOMO orbitals in the $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ molecule are localized in the triazine ring and a pyridine ring attached to this ring, while the LUMO orbitals are localized in the entire molecule except the ZnCl group. The energy difference between the HOMO-LUMO orbitals is an important parameter for conductivity [28,29]. This value in $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ molecule was calculated as 3.11 eV in gas phase. The difference between the frontier molecular orbitals in the solvent space of the molecule (acetonitrile) was calculated as 4.43 eV .

Table 7

The experimental and computed absorption wavelength λ (nm), excitation energies E (eV), absorbance and oscillator strengths (f) of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$.

Theoretical λ (nm)	E (eV)	f	Experimental λ (nm)	E (eV)
301.28 (104→114) $\pi \rightarrow \pi^n$	4.1152	0.0001	294	4.2172
285.08 (105→114) $\pi \rightarrow \pi^n$	4.3492	0.0718	289	4.2901

3.6.4. UV-Vis analysis

The electronic absorption spectrum of the complex molecule was calculated in the acetonitrile solvent by the TD-DFT / 6-311 (d, p) methods (nstates = 20). The absorption spectrum obtained was observed as a peak at 301 nm and a shoulder at 285 nm and it was drawn in Fig. 10. The wavelengths, excitation energies and electronic values of the molecule calculated for $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ molecule are given in Table 7. As can be seen from Table 7 and the spectrum, a peak at 289 nm and a shoulder at 294 nm were observed in the experimental spectrum. Excitation energies at the experimental wavelengths are given in the Table 7.

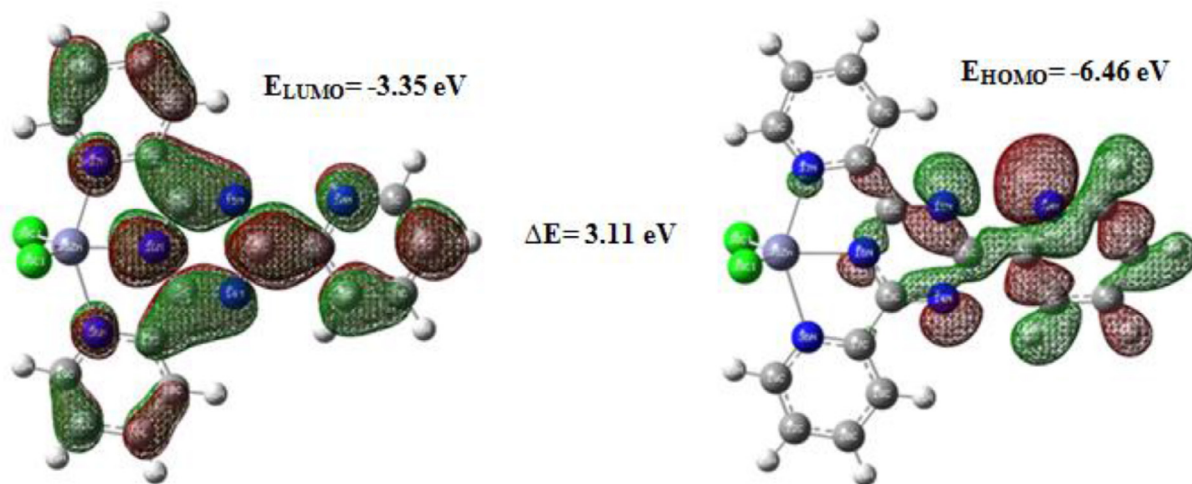


Fig. 9. The frontier molecular orbitals of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$.

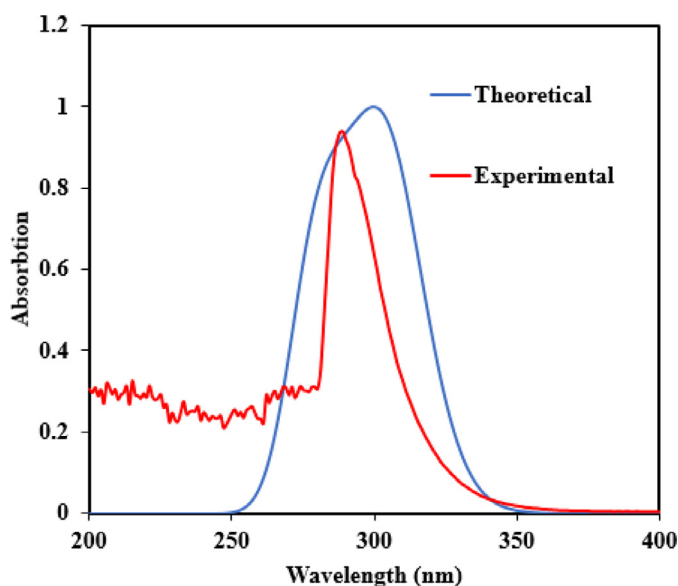


Fig. 10. Absorption spectra (theoretical and experimental) of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$.

4. Conclusion

In this work, $\text{Zn}(\text{II})$ complexes of 2,4,6-tris(2-pyridyl)-1,3,5-triazine ligand have been synthesized and fully characterized using various spectroscopic methods including single crystal X-ray diffraction. Molecular structure of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ was investigated by DFT, and one of the computational chemistry methods. In these calculations carried out in the gas phase, it was found to be in agreement with the experimental data of geometric parameters. It is revealed that the sharp peaks in the vibration spectrum of $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ calculated by the DFT method belong to the $\text{C}=\text{N}$ stretching band and these peaks are clearly observed experimentally in the complex molecule. When the electronic properties of the title molecule examined (HOMO-LUMO), gas phase, the energy difference (3.11 eV) than the value calculated in acetonitrile solvent (4.43 eV) it was observed to be smaller. $[\text{Zn}(\text{tptz})(\text{Cl})_2]$ has been found to show significant antimicrobial effects. It has been determined that it has significant effects especially on gram negative *P.aeruginosa*. Antibiotic resistance developing in gram negative bacteria in hospital flora is a major problem as a result of the use of many broad spectrum antibiotics in common and inappropriate

indications. The use of new methods and chemotherapeutics has become inevitable in combating species that cause hospital infections such as *P.aeruginosa*. Therefore, the antimicrobial effects of these newly synthesized chemicals can be investigated and used for new generation drugs. Complex didn't show any nuclease activity on pBR322 plasmid DNA absence of H_2O_2 . The percentage of nicked circular form increased in complex treated pBR322 DNA in the presence of H_2O_2 . Complex showed dose dependent nuclease activity by cutting DNA from a single strand in the presence H_2O_2 .

Credit author statement

Murat Çınarlı and Gamze Bakır Güven have carried out synthesis and characterization of the new compound. Emine Babur Şaş has carried out all theoretical studies. Önder İdil has carried out all experimental antimicrobial and DNA binding studies. Murat Çınarlı and Nermin Kehvecioğlu have read, edited and corrected the article.

Appendix A. Supplementary data

CCDC 1,841,037 contains the supplementary crystallographic data for $[\text{Zn}(\text{tptz})(\text{Cl})_2]$. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data center, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:[10.1016/j.molstruc.2021.130187](https://doi.org/10.1016/j.molstruc.2021.130187).

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