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### Detailed analytical studies of 1,2,4-triazole derivatized quinoline

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#### **RESEARCH ARTICLE**



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#### **KEYWORDS**

UV absorption Hirshfeld surface Cyclic voltammetry Single crystal structure Natural bond orbital (NBO) Time Dependent-Density Functional Theory

#### ABSTRACT

The present study describes, the X-ray single crystal analysis of 4-((2-chloro-6methoxyquinolin-3-yl)methyl)-2-phenyl-2H-1,2,4-triazol-3(4H)-one (TMQ). The crystal data for  $C_{19}H_{15}ClN_4O_2$ : monoclinic, space group  $P2_1/n$  (no. 14), a = 7.3314(15) Å, b = 12.459(3) Å, c = 18.948(4) Å,  $\beta = 98.322(9)^{\circ}$ , V = 1712.5(6) Å<sup>3</sup>, Z = 4, T = 296.15 K,  $\mu$ (MoK $\alpha$ ) = 0.245 mm<sup>-1</sup>, *Dcalc* =  $1.423 \text{ g/cm}^3$ , 5082 reflections measured ( $3.926^\circ \le 20 \le 38.556^\circ$ ), 1428 unique ( $R_{int} =$ 0.0545,  $R_{sigma} = 0.0574$ ) which were used in all calculations. The final  $R_1$  was 0.0423 (I  $>2\sigma(I)$  and  $wR_2$  was 0.1145 (all data). The Density functional theory optimized molecular geometries in TMQ agree closely with those obtained from crystallographic studies. The Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energy levels and energy gap were calculated by experimental (UV absorption & Cyclic voltammetry) and theoretical studies in two different solvents. The natural bond orbital analysis was performed to understand the molecular interaction on the basis of stability of molecule arising from hyper-conjugative interaction and charge delocalization. Hirshfeld surface and their related fingerprint plots enabled the identification of significant intermolecular interaction. The molecular electrostatic potential analysis provides the visual image of the chemically active sites and comparable reaction of atoms.

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#### 1. Introduction

Quinoline, an aza heterocycle, is pharmaceutically an important class of compound that exists as an emergence of pyridine ring and one benzene ring fused together at nearby two (side) carbon atoms [1]. These are widely used as a source compounds for the synthesis of numerous drugs. Many quinoline based drugs such as Captothecine (anticancer) [2] and Cryptolepine (antimalarial) [3] are available in the market. This skeleton also showed a broad spectrum of biological activities including antiasthmatic [4], antidiabetic [5], antibacterial [6], antitoxoplasma [7], antifungal [8] and anti-HIV [9] activities. Due to the presence of nitrogen, the quinoline moieties act as chelating agent as well as a weak base [10]. Some of thequinoline derivatives are often used as fluorescent materials and sensors due to their rigid structure, high fluorescent yield, and large energy gaps [11]. The 1,2,4-triazole scaffolds have attracted significant interest as chemotherapeutic agents, where they possess diverse pharmacological activities [12]. 1,2,4-Triazole nucleus is the main structural motif of many commercially available drugs including Fluconazole, Ribavirin, Letrozole and Itraconazole *etc.* [13-15].

4-((2-Chloro-6-methoxyquinolin-3-yl)methyl)-2-phenyl-2*H*-1,2,4-triazol-3(4*H*)-one (TMQ) was designed and molecular docking study was performed to explore the mechanism of anti-TB as well as anticancer activity and to study the intermolecular interactions between the targeted enzyme (Enoyl-acyl carrier protein) and TMQ. Based on impressive outcome of docking study (C-Score = 5.89) of the TMQ, the molecule was synthesized structure was characterized. Further, *invitro* study was carried out and it was found that this molecule is promising candidate for developing novel anticancer (GI<sub>50</sub> = 63.15 μM) and anti-tubercular (MIC<sub>90</sub> = 0.100 μM) agent [16].

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Table 1. Summary of the crystal structure, data collection, and crystallographic refinement data of TMQ.

Parameter	Values	
Empirical formula	$C_{19}H_{15}ClN_4O_2$	
Formula weight	366.80	
Temperature (K)	296.15	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 <sub>1</sub> /n	
a (Å)	7.3314(15)	
b (Å)	12.459(3)	
c (Å)	18.948(4)	
β (°)	98.322(9)	
Volume (ų)	1712.5(6)	
Z	4	
$\rho_{calc}(g/cm^3)$	1.423	
μ(mm <sup>-1</sup> )	0.245	
F(000)	760.0	
Crystal size (mm <sup>3</sup> )	$0.15 \times 0.12 \times 0.11$	
Radiation	ΜοΚα (λ = 0.71073)	
20 range for data collection (°)	3.926 to 38.556	
Index ranges	$-5 \le h \le 6, -11 \le k \le 10, -17 \le l \le 16$	
Reflections collected	5082	
Independent reflections	1428 [ $R_{int} = 0.0545$ , $R_{sigma} = 0.0574$ ]	
Data/restraints/parameters	1428/0/236	
Goodness-of-fit on F <sup>2</sup>	1.021	
Final R indexes [I≥2σ (I)]	$R_1 = 0.0423$ , $wR_2 = 0.1029$	
Final R indexes [all data]	$R_1 = 0.0588$ , $wR_2 = 0.1145$	
Largest diff. peak/hole (e.Å-3)	0.23/-0.19	
CCDC deposition number	1828103	

The structural, spectroscopic and photophysical behavior of a molecule depends on function of its overall molecular structure and hence there is a scope in the synthesis of novel conjugate molecules by combining two different moieties together and studying their properties [17]. Also, the spectroscopic and structural behaviors of various molecules using both experimental and theoretical methods have fascinated the curiosity of researchers for many years. Density functional theory (DFT) has become a very useful tool for theoretical calculation in current years. The theoretical calculations using DFT have been utilized to study molecular properties such as structural, spectroscopic and photophysical properties [18-21]. DFT is computationally less challenging than wave function as it also expresses small molecules more reliably than Hartree-Fock theory [22,23].

In the present work, a combined approach by X-ray crystallography (XRD) and DFT calculation was handled, which takes the benefit of both the reliability of the experimental technique and high interpretative influence of the theoretical studies and the accuracy. The structural confirmation was done by XRD data. Since, X-ray diffraction study has become indispensable device in crystal chemistry as it assists in solving the molecular structure, magnitudes and directional characteristics. The exact results of molecular structure of compound TMQ will become important due to experimental facts which help in designing molecules for potential pharmacological property. The theoretical structural predicttions have been carried out by using density functional theory. Ultraviolet (UV)-Visible spectra of TMQ in gaseous phase, ethanol, and acetonitrile are simulated using the Time-dependent density functional theory (TD-DFT). The HOMO and LUMO are analyzed to describe the electronic transition properties of the systems investigated. The theoretically predicted UV Visible spectra of TMQ are compared with the observed experimental results, and discussed. The HOMO and LUMO are also determined by using cyclic voltammetry technique and these are in good agreement with the theoretical results. The general structural features and to predict the reactivity of a molecule, natural bond orbital (NBO) analysis has been carried out which provides important information regarding orbital interactions and electron density among them [24].

#### 2. Experimental

2.1. Synthesis

4-((2-Chloro-6-methoxyquinolin-3-yl)methyl)-2-phenyl-2H-1,2,4-triazol-3(4H)-one was synthesized according to reported method [16]. TMQwas dissolved in DMSO and heated until the moisture is eliminated. The saturated solution was filtered through the Whatman filter paper into a clean and dry beaker and kept aside for slow evaporation for a period of 15 days at room temperature. Purple colored rectangular shaped crystals of TMQwere collected. Good diffraction quality single crystals were studied further for structural analysis.

#### 2.2. X-ray crystallography

A single crystal of dimensions 0.11 × 0.12 × 0.15 mm of TMQ was chosen for X-ray diffraction study. The X-ray intensity data were collected at a temperature of 293 K on a Rigaku Saturn724 diffractometer using graphite monochromated  $MoK_{\alpha}$  radiation. A complete data set was processed using CrystalClear [25]. The structure was solved by direct method and refined by full-matrix least squares method on  $F^2$ using SHELXS and SHELXL programs [26]. All the nonhydrogen atoms were revealed in the first difference Fourier map itself. All the hydrogen atoms were positioned geometrically and refined using a riding model. After ten cycles of refinement, the final difference Fourier map showed peaks of no chemical significance. The geometrical calculations were carried out using the program PLATON [27]. The molecular and packing diagrams were generated using the software MERCURY [28]. The details of the crystal structure and data refinement are given in Table 1. The ORTEP [28] of the molecule with thermal ellipsoids are drawn at 50%probability is shown in Figure 1.

#### 2.3. Hirshfeld surface calculations

Three-dimensional (3D) molecular Hirshfeld surfaces and the two-dimensional (2D) fingerprint plots represent a new way of visualizing and analysing intermolecular interactions in molecular crystals, and are basically different from conventional methods of crystal structure analysis. The molecular Hirshfeld surface [29] in the crystal of organic compounds is created by dividing space in the crystal into regions where the electron distribution as the sum of atoms for the molecule dominates the corresponding sum over the crystal.

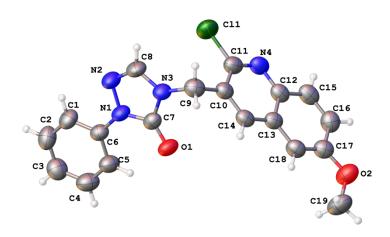


Figure 1. ORTEP of TMQ showing the atomic numbering system. Displacement ellipsoids are drawn with 50% probability.

Hirshfeld surfaces and their related fingerprint plots are generated using the program Crystal Explorer 3.0 [30]. The crystallographic information file (.cif) is given as input to the Crystal Explorer program. The Hirshfeld surface is unique for a given crystal structure and for a set of spherical atomic electron densities. Each point on the Hirshfeld surface is specified with two distances: the distance from the Hirshfeld surface to the nearest nucleus inside the surface is *d* and to the nearest nucleus outside the surface is  $d_e$ . Then  $d_{norm}$  is the normalized contact distance which is defined in terms of  $d_{i_i}$  $d_e$  and the van der Waals radii (vdW) of the atoms. The electrostatic potential is mapped on Hirshfeld surface using STO-3G (Slater-type-orbitals simulated by 3 Gaussians) basis set at the Hartree-Fock theory over the range -0.069 au (red), through 0 (white) to 0.043 au (blue). Crystal geometries were used as input to the TONTO [31] integrated with Crystal Explorer. The acceptor atoms in these interactions are shown with negative electrostatic potentials (red regions) and donor atoms are shown with positive electrostatic potentials (blue regions) [32].

#### 2.4. UV absorption spectroscopy

Absorption spectra of TMQ was recorded using UV-Vis, NIR (JASCO V-670, Japan) spectrophotometer at room temperature, keeping the concentrations of compound  $1 \times 10^{-5}$  M in ethanol and acetonitrile.

#### 2.5. Cyclic voltammetry (CV)

Cyclic voltammetry (CV) study of TMQ was carried out using an Electrochemicalanalyzer / Work station (model 600E series, USA) at room temperature. CV consists of three electrode system that is Ag/AgCl reference electrode (RE), platinum counter electrode (CE) and glassy carbon working electrode (WE). The CV measurements of TMQ ( $1 \times 10^{-3}$  M concentration) were obtained at 0.1 M with tetrabutyl ammonium perchlorate as supporting electrolyte in dimethylsulphoxide (Acetonitrile) solvent with a scan rate 100 mV/s.

#### 2.6. Density functional theory (DFT) calculations

The DFT calculations were performed using Gaussian 09 software package [33]. The potential energy surface scan has been carried out with (Hartree-Fock) HF/6-31G level to place the molecule at local minima. The geometry at local minima has been assumed as starting point for the calculation by utilizing Becke's three parameter hybrid model with the Lee-

Yang-Parr correlation functional (B3LYP) method [34,35]. The geometry is optimized with 6-31++G(d,p) and 6-311++G(2d,p) basis sets for comparison with XRD data. The HOMO ( $E_{HOMO}$ ), LUMO ( $E_{LUMO}$ ) energy levels and energy gap ( $E_g$ ) were calculated by TD-DFT in gas phase and in two different solvents using 6-311++G(2d,p) basis set. The NBO analysis was performed using NBO 3.1 program [36] as implemented in the Gaussian 09 package at the DFT/B3LYP level using 6-311++G(2d,p) basis set. The molecular electrostatic potential surfaces (MEPs) and the Mulliken charge distributions of the title molecule were obtained from the population analysis calculations and visualized using Gauss View 5 [37].

#### 2.7. Molecular electrostatic potential

The molecular electrostatic potential (MEP) surface was determined by DFT level in order to know the relative polarity of the molecule. MEP is formed by the nuclei and the electrons (treated as static distribution of charge) and is typically visualized through its values on the molecular electron density. MEP mapping is very helpful descriptor in understanding sites for relative reactivity towards electrophilic and nucleophilic [38] attacks, in studies of biological identification as well as hydrogen bonding interactions [39,40]. The electrostatic potential V(r) has been mainly useful as sign of the regions or sites of a molecule to which an approaching electrophile is primarily attracted, and is also well matched for analyzing processes based on the "recognition" of one molecule by another, as in enzyme-substrate, drug-receptor, and interactions, since it is through their potentials that the two species initially "see" each other [41,42].

#### 3. Results and discussion

#### 3.1. Description of the crystal structure

The ORTEP of TMQ with thermal ellipsoids are drawn at 50% probability shown in Figure 1. The title molecule crystallizes in monoclinic crystal system (space group  $P2_1/n$ ) with unit cell dimensions a = 7.3314(15) Å, b = 12.459(3) Å, c = 18.948(4) Å,  $\beta = 98.322(9)^{\circ}$  and Z = 4. Crystallographic data, details of the data collections and structure refinement parameters of the compoundTMQ were determined. The resulted all bond lengths, bond angles and dihedral angles are in good agreement with the calculated values, and tabulated in Tables 2-4, respectively.

Atoms         Experimental         Calculated (B3/P/6-31 + + G(dg))         Calculated (B3/P/6-311 + + G(dg))           07-01         1.358         1.358         1.358           07-01         1.358         1.358         1.358           07-01         1.354         1.358         1.359           07-01         1.354         1.229         1.239           07-01         1.354         1.229         1.238           07-01         1.374         1.229         1.448           07-01         1.374         1.229         1.448           07-01         1.374         1.422         1.448           07-01         1.374         1.421         1.448           07-01         1.346         1.449         1.441           07-01         1.346         1.441         1.441           07-01         1.3465         1.349         1.347           07-01         1.3465         1.342         1.441           07-01         1.347         1.441           07-01         1.347         1.441           07-01         1.347         1.443         1.442           07-01         1.347         1.342         1.347           07-01 </th <th>Table 2. Experimental and cal</th> <th></th> <th></th> <th></th>	Table 2. Experimental and cal			
02-019         1.428[0]         1.425         1.422           02-017         1.358[0]         1.364         1.238           M-C11         1.249[0]         1.299         1.201           01-07         1.359[0]         1.387         1.385           N-42         1.397[0]         1.387         1.385           N-46         1.412[0]         1.429         1.418           N-46         1.412[0]         1.383         1.375           C17-C16         1.400[0]         1.383         1.375           C17-C16         1.403[5]         1.422         1.411           C17-C16         1.403[5]         1.422         1.412           C17-C16         1.403[5]         1.422         1.411           C12-C12         1.411[0]         1.417         1.411           C12-C12         1.410[0]         1.422         1.411           C12-C12         1.410[0]         1.422         1.422           C12-C13         1.492[0]         1.433         1.422           C12-C1         1.379[0]         1.394         1.399           C2-C1         1.379[0]         1.392         1.394           C2-C1         1.379[0]         1.394         <		Experimental	Calculated (B3LYP/6-31 ++G(d,p))	Calculated (B3LYP/6-311 ++G(2d,p))
02-C171.358(5)1.3611.358N4-C121.354(5)1.2991.291N4-C121.354(6)1.3621.359N4-C71.374(5)1.3871.386N1-C71.374(5)1.3891.386N1-C61.427(5)1.4221.448N2-C61.275(6)1.3821.201N2-C71.374(5)1.3821.201N2-C81.275(6)1.4221.441C7-C81.407(5)1.4221.411C13-C121.411(5)1.4271.411C13-C121.411(5)1.4271.411C13-C121.411(5)1.4271.421C14-C101.381(5)1.3821.302C14-C101.381(5)1.3821.302C14-C101.381(5)1.3821.302C14-C101.381(5)1.3821.306C14-C101.387(6)1.3921.306C14-C101.387(5)1.3971.393C4-C21.367(5)1.3961.399C4-C31.362(5)1.3961.399C4-C31.362(5)1.3961.399C4-C41.375(5)1.3971.386C4-C41.375(5)1.3971.386C4-C41.362(5)1.3971.398C4-C31.362(5)1.3971.398C4-C41.364(5)1.3971.398C4-C41.375(5)1.3971.398C4-C41.362(5)1.3981.399C4-C41.364(5)1.398<		1.742(4)		
N-C11         1.294         1.291           N-C12         1.35461         1.353         1.357           N-C4         1.35561         1.387         1.358           N-C5         1.412         1.418         1.357           N-C6         1.41251         1.422         1.418           N-C6         1.41251         1.422         1.418           N-C6         1.41251         1.422         1.418           C7-C16         1.40515         1.358         1.375           C37-C16         1.40515         1.422         1.410           C37-C17         1.41051         1.427         1.411           C4-C10         1.35851         1.351         1.311           C4-C10         1.35851         1.352         1.351           C4-C11         1.41051         1.426         1.420           C4-C2         1.35751         1.342         1.426           C4-C3         1.35751         1.342         1.346           C4-C4         1.37951         1.342         1.416           C5-C4         1.37951         1.342         1.416           C5-C4         1.37951         1.342         1.416           C5-C1		1.420(5)	1.425	1.422
N-C12         1.354(4)         1.363         1.359           OL-C7         1.254(4)         1.239         1.239           N1-R6         1.355(4)         1.387         1.388           N1-R6         1.425(5)         1.429         1.438           N1-R6         1.425(5)         1.429         1.438           N2-G6         1.426(5)         1.421         1.431           N2-G7         1.440(5)         1.442         1.441           C17-C16         1.442(5)         1.442         1.441           C14-C17         1.441         1.441(5)         1.442           C14-C10         1.538(5)         1.535         1.511           C14-C10         1.538(5)         1.339         1.3367           C14-C11         1.416(5)         1.442         1.349           C14-C11         1.416(5)         1.442         1.349           C14-C11         1.416(5)         1.442         1.349           C14-C11         1.416(5)         1.442         1.349           C14-C1         1.357(5)         1.443         1.399           C14-C1         1.357(6)         1.342         1.340           C14-C1         1.379(6)         1.398	02-C17	1.358(5)	1.361	1.358
0-C7         1.215(4)         1.229         1.220           NH-R2         1.355(4)         1.389         1.385           NL-C7         1.374(5)         1.389         1.385           NL-C7         1.374(5)         1.489         1.385           C7-C16         1.464(5)         1.420         1.420           C7-C16         1.464(5)         1.422         1.411           C17-C16         1.442(5)         1.420         1.420           C13-C14         1.401(5)         1.427         1.411           C14-C10         1.441(5)         1.427         1.431           C14-C10         1.441(5)         1.426         1.420           C14-C10         1.441(5)         1.426         1.430           C14-C20         1.326(5)         1.338         1.3397           C14-C21         1.326(5)         1.339         1.3397           C4-C2         1.326(5)         1.339         1.3397           C4-C3         1.326(5)         1.339         1.3397           C4-C4         1.379(5)         1.339         1.339           C4-C3         1.326(5)         1.339         1.349           C17-C10         1.364(5)         1.339	N4-C11	1.294(5)	1.299	1.291
Ni-R2     1.386/4)     1.387     1.385       Ni-C6     1.42(5)     1.422     1.418       Ni-C6     1.42(5)     1.422     1.418       Ni-C6     1.42(5)     1.422     1.418       C12-C16     1.463(5)     1.422     1.416       C13-C12     1.441(5)     1.425     1.420       C13-C12     1.41(5)     1.427     1.416       C13-C12     1.41(5)     1.427     1.421       C14-C10     1.348(5)     1.387     1.372       C14-C10     1.348(5)     1.387     1.395       C4-C3     1.452(4)     1.463     1.460       C4-C3     1.352(4)     1.372     1.397       C4-C3     1.352(4)     1.372     1.397       C4-C3     1.352(5)     1.403     1.397       C4-C3     1.352(5)     1.398     1.399       C4-C3     1.362(5)     1.398     1.399       C3-C2     1.364(5)     1.372     1.398       C12-C15     1.404(5)     1.425     1.461       C12-C15     1.404(5)     1.425     1.461       C12-C16     1.394(5)     1.398     1.398       C12-C16     1.394(5)     1.398     1.398       C12-C16     1.394(5)     <	N4-C12	1.354(4)	1.363	1.359
Ni-R2         1.387         1.387         1.386           Ni-C6         1.4225         1.422         1.418           Ni-C6         1.4225         1.422         1.418           Ni-C6         1.4215         1.422         1.418           C17-C16         1.40515         1.422         1.416           C17-C16         1.40615         1.442         1.416           C13-C12         1.4115         1.427         1.416           C13-C12         1.4115         1.427         1.416           C14-C10         1.5813         1.383         1.371           C14-C10         1.5813         1.383         1.395           C14-C10         1.4105         1.463         1.460           C14-C10         1.4315         1.463         1.460           C14-C10         1.4351         1.463         1.460           C4-C3         1.3551(1)         1.372         1.360           C4-C3         1.362(5)         1.397         1.399           C4-C3         1.364(5)         1.372         1.360           C12-C1         1.756(4)         1.4841         1.462           C12-C1         1.364(5)         1.374         1.360     <	01-C7	1.215(4)	1.229	1.220
N1-C71.374(5)1.3891.386N2-C61.42(5)1.42(2)1.418N2-C81.275(4)1.2981.291N2-C81.40(5)1.3381.376C17-C181.40(5)1.4221.411C13-C141.40(15)1.4221.411C13-C121.411(5)1.4271.421C13-C141.401(5)1.4471.421C14-C101.536(5)1.5151.511C14-C101.536(5)1.5151.511C14-C101.337(5)1.4021.367C6-C31.357(5)1.4021.367C6-C41.377(5)1.4021.367C5-C41.377(5)1.4021.396C5-C41.377(5)1.4021.306C5-C41.375(5)1.3971.306C2-C11.375(5)1.3981.391C2-C21.345(5)1.3341.381C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.386C2-C11.375(5)1.3941.396C2-C11.375(5)1.3941.396C2-C11.375(5)1.3941.396C2-C11.375(5)1.3941.396C2-C11.375(5)1.3941.396C2-C11.375(5)1.394	N1-N2			
N1-C6         142[5]         1422         1418           N2-C6         125(4)         129         1376           C17-C16         136(5)         1333         1376           C17-C16         1407(5)         1427         1441           C18-C14         1407(5)         1427         1441           C18-C12         1411(5)         1427         1441           C14-C10         1358(5)         1382         1375           C16-C9         152(2)         1515         1511           C16-C9         152(5)         1393         1397           C16-C3         137(4)         1398         1397           C6-C3         137(5)         1402         1306           C5-C4         137(5)         1397         1397           C6-C3         136(5)         1396         1399           C2-C2         136(15)         1398         1396           C2-C2         136(15)         1397         1398           C2-C2         136(15)         1397         1398           C2-C2         136(15)         1397         1398           C2-C2         136(15)         1397         1398           C2-C2 <td< td=""><td>N1-C7</td><td></td><td></td><td></td></td<>	N1-C7			
N2-081275[4]12881291C77-C181406[5]13831376C77-C181405[5]14221446C17-C181407[5]14221416C13-C121411(5]14271431C13-C121411(5]14271431C14-C101535[5]15351511C14-C101535[5]15351511C16-C111440[5]14621440C0-C11572[4]13921397C0-C31377[5]14031397C6-C31367[5]14021396C5-C41375[5]13971390C5-C41362[5]13961391C5-C41355[5]13921391C5-C41355[5]13921391C5-C41355[5]13921391C5-C41375[5]13941381C5-C41375[5]13921381C5-C41375[5]13941381C5-C41375[5]13941381C5-C51374[6]185518271C6-C11141[3]11174511154C7-C41143[3]11274C11441144[3]14421C11441144[3]14421C11441144[3]14421C11441144[3]114519C11441144[3]114519C11441249[6]12512C217-C161144[4]11429C11441249[6]1209[6]C114412249[6]				
C17-C161.360(5)1.3831.376C17-C161.440(5)1.4421.440C18-C131.407(5)1.4221.411C13-C141.401(5)1.4271.421C13-C121.411(5)1.4271.421C10-C71.501(5)1.4271.421C10-C71.501(5)1.4271.421C10-C71.52(4)1.4261.423C10-C71.52(4)1.4361.460N3-C71.372(4)1.3981.395N3-C81.35(4)1.3721.307C4-C31.337(5)1.3961.399C4-C31.336(5)1.3961.399C4-C41.374(5)1.3961.391C2-C21.361(5)1.3961.391C2-C41.374(5)1.3941.391C2-C41.375(5)1.3941.391C2-C41.375(5)1.3941.391C2-C41.375(5)1.3941.391C2-C41.375(5)1.3941.391C2-C41.374(5)1.3941.381C2-C41.374(5)1.3941.381C2-C41.374(5)1.3941.391C2-C41.374(5)1.3941.391C2-C41.374(5)1.3941.391C2-C51.444(5)1.4441.445C2-C41.374(5)1.3641.362C1-74-C41.374(5)1.3641.364C1-72-C51.3941.3241.324C1-72-C61.994(4)1.2243 <td></td> <td></td> <td></td> <td></td>				
C17-C161443[5]14251420C18-C131407(5)14221416C13-C121411(3)14471411C13-C121413(3)14271421C14-C10138(6)13821375C14-C10138(6)13821375C14-C10138(6)14421372C9-N31452(4)14631460N3-G71372(4)13981395N3-G81355(4)14021396C4-C2137(5)14021396C4-C3137(6)14021396C4-C4137(6)13721396C4-C51361(7)13721367C4-C4137(5)13721366C12-C151384(8)14221416C12-C151354(8)13721368C12-C161354(8)1182751368C17-02-C161354(8)1182751466C17-02-C171168(3)11827511663C17-02-C181254(4)11827511663C17-02-C191168(3)1182711674C17-02-C191168(3)11827511663C17-02-C191168(3)11827511663C17-02-C191168(3)11827511663C17-02-C191168(3)11827511674C17-02-C191168(3)11827511663C17-02-C191126(4)11627611674C17-02-C191126(4)11627611674C17-02-C191126(4)116276 <td></td> <td></td> <td></td> <td></td>				
C18 C13         1407(2)         1422         1416           C13 C14         1401(5)         1427         1421           C14 C10         1389(5)         1382         1375           C14 C10         1389(5)         1382         1375           C14 C10         1389(5)         1382         1375           C14 C11         1410(3)         1424         1420           N3-67         1372(4)         1393         1395           N3-68         1355(4)         1372         1367           C6-C3         1367(5)         1403         1397           C5-C4         1379(5)         1402         1396           C4-C2         1364(5)         1392         1396           C4-C3         1342(5)         1397         1398           C4-C3         1342(5)         1392         1391           C4-C4         1354(6)         1422         1416           C4-C4         1354(7)         1392         1392           C4-C2         1354(7)         1428         1416           C4-C2         1276(4)         118491         1182           C14-C4         1276(4)         118491         1182           C14-C4 </td <td></td> <td></td> <td></td> <td></td>				
C13-C12         1.410         1.417         1.411           C13-C12         1.4116)         1.427         1.421           C14-C10         1.358(5)         1.382         1.375           C10-C9         1.552(5)         1.511         1.426           C14-C11         1.410(5)         1.426         1.420           C14-C1         1.410(5)         1.426         1.420           NS-C         1.372(6)         1.402         1.397           C4-C3         1.377(5)         1.402         1.390           C4-C3         1.362(5)         1.396         1.391           C2-C2         1.361(5)         1.392         1.365           C2-C1         1.375(5)         1.402         1.365           C2-C1         1.375(5)         1.492         1.416           C2-C1         1.375(5)         1.492         1.365           C2-C1         1.159(4)         1.2009         1.20134				
C13-C121.411(5)1.4271.421C14-C101.358(5)1.5151.517C10-C91.552(5)1.5151.511C9-N31.452(4)1.4631.460C9-N31.452(4)1.4631.460C9-N31.452(4)1.4631.460C9-C31.357(5)1.4031.397C6-C31.357(5)1.4021.396C5-C41.379(5)1.4021.396C5-C41.379(5)1.4021.398C5-C41.379(5)1.3981.391C5-C41.354(5)1.3981.391C5-C41.354(5)1.3921.388C5-C41.354(5)1.3941.388C5-C41.354(5)1.3941.388C5-C41.354(5)1.3921.388C5-C41.354(5)1.3921.388C5-C41.354(5)1.3921.388C5-C41.354(5)1.3921.388C5-C41.354(5)1.3921.388C5-C41.354(5)1.8551.8630C7-C151.56(4)1.82551.8630C7-N1-N21.164(3)1.10041.8630C7-N1-N21.153(4)1.82041.2628C7-N1-N21.153(4)1.20041.2028C7-N1-N21.153(4)1.20041.2028C7-N1-N21.153(4)1.20041.2028C7-N1-N21.153(4)1.20041.2028C7-N1-N21.204(4)1.20041.2028C7-N1-N2 <t< td=""><td></td><td></td><td></td><td></td></t<>				
C14-C10         1.586[5]         1.582         1.575           C10-C9         1.520[5]         1.515         1.511           C10-C9         1.420[7]         1.420         1.420           C0-N3         1.425[7]         1.463         1.420           N3-C7         1.327[4]         1.398         1.397           C6-C1         1.375[5]         1.402         1.396           C6-C4         1.375[5]         1.397         1.390           C6-C4         1.375[5]         1.398         1.391           C12-C5         1.406[5]         1.398         1.391           C12-C15         1.406[5]         1.392         1.365           C2-C1         1.375[5]         1.394         1.385           C2-C1         1.375[5]         1.394         1.385           C2-C1         1.375[5]         1.394         1.385           C2-C1         1.375[5]         1.394         1.385           C2-C2         1.36[5]         1.388         1.391           C2-C2         1.36[5]         1.383         1.385           C2-C1         1.575[6]         1.384         1.381           C2-C2         1.58[5]         1.383         1.555 <td></td> <td></td> <td></td> <td></td>				
C10-C91502(5)1.5151.5171.420C0-N31.422(4)1.4631.460N3-C71.327(4)1.3981.395N3-C81.355(4)1.3721.367C4-C11.377(5)1.4031.397C5-C11.377(5)1.4021.396C5-C21.367(5)1.4021.396C5-C31.377(5)1.3961.399C4-C41.367(5)1.3961.399C5-C41.377(5)1.3941.393C5-C41.354(5)1.3721.365C2-C11.354(5)1.3721.365C2-C11.354(5)1.3721.365C17-02-C191.66(3)118.555118.630C17-02-C191.66(3)118.91118.275C17-02-C191.166(3)118.91118.275C17-02-C191.15(4)120.099120.134C17-02-C191.06(3)112.009120.134C7-N1-C61.91(4)120.091120.134C7-N1-C61.91(4)120.091120.134C7-N1-C61.99(4)120.134120.134C7-N1-C61.99(4)120.134120.134C17-C16-C11.99(4)120.63120.144C18-C12-C21.20.3(4)120.64120.99C14-C13-C121.74(4)116.056160.90C14-C13-C121.74(4)116.056160.90C14-C13-C121.74(4)120.64120.99C14-C13-C121.74(4)120.64120.299C14				
Cl0-Cl11         1.410[5]         1.426         1.460           N3-C7         1.372(4)         1.398         1.395           N3-C8         1.355(4)         1.372         1.367           6-C5         1.367(5)         1.403         1.397           6-C6         1.367(5)         1.402         1.396           C5-C4         1.379(5)         1.396         1.389           C3-C2         1.361(5)         1.398         1.391           C3-C4         1.357(5)         1.396         1.389           C3-C2         1.361(5)         1.394         1.398           C4-C1         1.357(5)         1.394         1.389           C4-C1         1.357(5)         1.394         1.389           C4-C1         1.357(5)         1.394         1.388           C4-C1         1.357(5)         1.394         1.338           C4-C1         1.364(3)         1.422         1.431           C17-O2C19         1.66(2)         1.8491         1.8215           C17-O2C19         1.66(2)         1.8491         1.8236           N2-N1-C6         1.91(4)         1.28243         1.8281           N2-N1-C6         1.924(4)         1.2056				
CP-N31.452[4]1.4631.460N3-C71.357(4)1.3981.395N3-C81.355(4)1.3721.367C6-C11.379(5)1.4021.396C6-C21.367(5)1.4021.396C6-C31.362(5)1.3971.390C4-C31.362(5)1.3921.391C4-C31.362(5)1.3921.391C4-C41.375(5)1.3921.396C4-C51.375(5)1.3921.386C4-C11.375(5)1.3921.386C4-C21.375(5)1.3941.8275C4-C11.375(5)1.3941.8275C17-02-C191.66(3)1.184911.8275C17-02-C191.66(3)1.184911.8275C17-02-C191.66(3)1.184911.8275C17-02-C191.66(3)1.184911.8275C17-02-C191.66(3)1.184911.8275C17-02-C191.56(3)1.128431.8275C17-02-C191.56(3)1.128431.8271C17-02-C191.52(4)1.220091.2014C7-N1-661.94(4)1.84511.8271C7-N1-661.94(4)1.82431.8271C2-C1-C161.14(4)1.44681.4519C17-C161.44(4)1.44681.4519C17-C161.94(4)1.24641.26061C17-C161.94(4)1.24661.9901C17-C161.94(4)1.24661.9901C17-C161.94(4)1.26061 <td></td> <td></td> <td></td> <td></td>				
N2-C71.372[4]1.3961.395N2-C81.367(5)1.4031.397C6-C51.367(5)1.4021.396C5-C41.379(5)1.3971.390C5-C41.379(5)1.3961.399C4-C31.362(5)1.3961.399C4-C21.361(5)1.3981.391C2-C11.375(5)1.3941.306C2-C11.375(5)1.3941.308Table 3. Experimental and calculated boot angles (*) for TMQ.Table 3. Experimental and calculated boot angles (*) for TMQ.Table 3. Experimental and calculated (*) for TMQ.Calculated (*) for TMQ.				
N3-68         1.357(i)         1.472         1.367           C6-C5         1.379(5)         1.403         1.397           C6-C1         1.379(5)         1.396         1.396           C5-C4         1.379(5)         1.397         1.396           C4-C3         1.362(5)         1.398         1.391           C12-C1         1.361(5)         1.372         1.365           C2-C1         1.375(5)         1.394         1.388           C2-C1         1.375(5)         1.394         1.388           C2-C1         1.375(5)         1.394         1.388           C2-C1         1.375(5)         1.394         1.388           C2-C1         1.375(5)         1.8491         1.8275           C1-N4-C2         17.5(4)         118.55         1.186.63           N2-N1-C6         119.1(4)         120.009         1.2184           C7-N1-R2         11.3(3)         11.745         1.1594           C7-N1-R2         11.3(3)         1.1594         1.56           C7-N1-R2         11.3(3)         1.1594         1.56           C7-N1-R2         11.3(3)         1.1594         1.56           C7-N1-R2         119.9(4)         120.049<				
C6C5         1.307(5)         1.403         1.397           C5C4         1.379(5)         1.397         1.396           C5C4         1.379(5)         1.396         1.389           C4C3         1.362(5)         1.396         1.389           C3C2         1.361(5)         1.398         1.391           C12C15         1.408(5)         1.422         1.416           C12C15         1.384(5)         1.372         1.365           C1402         1.375(5)         1.394         1.388           Table 3. Experimental and calculated (B3LVP/6-31 ++6(d.p.))         Calculated (B3LVP/6-31 ++6(d.p.))           C17-02-C19         116.6(3)         118.491         118.275           C17-02-C19         116.6(3)         118.491         118.275           C17-02-C19         116.6(3)         116.491         118.491           C17-02-C19         115.6(3)         113.491         11.495           C17-02-C19         115.6(3)         115.94         126.191           C7-N1-C6         119.4(4)         114.486         145.191           C2-C17-C16         119.4(4)         114.486         145.191           C16-C1-C16         119.9(4)         120.512         120.5161     <				
C6C1         1.379(5)         1.402         1.396           C5C4         1.379(5)         1.397         1.390           C4C3         1.362(5)         1.396         1.391           C12C15         1.408(5)         1.422         1.416           C15C16         1.375(5)         1.394         1.388           Table 2.         Experimental and calculated boar angles (*) for TMQ.         1.388           Table 3.         Experimental and calculated (B3LVP/6-31 ++6(d.p.))         Calculated (B3LVP/6-31 ++6(d.p.))           C17-02C19         116.8(3)         118.491         118.275           C11-N4-C12         117.5(4)         118.555         118.630           N2-N1-C6         119.1(4)         120.009         120.134           C7-N1-A2         11.3(3)         11.745         111.594           C7-N1-A2         11.2(3)         120.009         120.134           C7-N1-C6         129.4(4)         128.243         128.271           C8-N2-N1         104.0(3)         105.004         105.007           C2-C1-C16         119.9(4)         120.291         122.968           C1-C1C4         129.4(4)         120.491         120.591           C1-C1C41         120.4(4)         120.664 <td></td> <td></td> <td></td> <td></td>				
C5-C4         1.379         1.390           C4-C3         1.362(5)         1.396         1.391           C3-C2         1.361(5)         1.392         1.391           C12-C15         1.400(5)         1.422         1.416           C12-C15         1.354(5)         1.324         1.388           Toble 3. Experimental and c20/est of pr TMQ.         1.388         1.388           Toble 3. Experimental and c20/est of pr TMQ.         1.384         1.88.30           C17-02-C19         116.8(3)         118.491         118.630           C17-02-C19         116.8(3)         117.45         118.630           C7-N1-C6         119.1(4)         128.243         128.271           C7-N1-C6         119.4(4)         114.466         114.519           C7-C1-C18         125.6(4)         125.123         125.192           C2-C17-C16         114.4(4)         114.466         114.519           C18-C17-C16         114.4(4)         114.519         120.288           C17-C16         114.4(4)         120.636         120.041           C14-C13-C1         120.3(4)         120.64         120.64           C14-C14-C1         120.3(4)         120.66         16.990           C				
C4-C3         1.362(5)         1.396         1.389           C3-C2         1.361(5)         1.398         1.391           C12-C15         1.408(5)         1.322         1.365           C2-C1         1.375(5)         1.394         1.388           Table 3.Experimental calc/later borned         Calculated (B3LVP/6-31 ++6(d.p.)         Calculated (B3LVP/6-31 ++6(d.p.))           C17-02 C19         116.6(3)         118.491         118.275           C11-N-C12         117.5(4)         118.555         118.630           N2-N1-C6         119.1(4)         120.009         120.134           C7-N1-N2         111.3(3)         11.745         111.594           C7-N1-C6         129.4(4)         128.234         128.271           C7-N1-C6         129.4(4)         120.309         120.144           C7-N1-C6         119.9(4)         120.391         120.288           C7-C1-C16         119.9(4)         120.391         120.241           C17-C216         129.4(4)         120.666         120.041           C14-C13-C12         120.3(4)         120.661         120.61           C14-C13-C12         120.8(4)         120.661         120.61           C14-C14-C13         120.8(4)				
C3-C2         1.361(5)         1.398         1.391           C12C15         1.400(5)         1.422         1.416           C15C16         1.354(5)         1.372         1.365           C2-C1         1.375(5)         1.394         1.388           Table 3. Experimental and calculated bond angles (*) for TNQ.         Calculated (B3LYP/6-31++6(d.pl))         Calculated (B3LYP/6-31++6(d.pl))         Calculated (B3LYP/6-31++6(d.pl))           C17-02-C19         115.64(3)         118.491         18.275         118.610           C7-N1-C6         119.1(4)         112.55         118.610         11.544           C7-N1-C6         119.1(4)         112.624         111.54           C7-N1-C6         12.94(4)         12.8243         128.271           C8-N2-N1         104.0(3)         105.004         105.007           C2-C17-C16         11.44(4)         114.466         114.519           C2-C17-C16         11.54(4)         112.55         113.611           C18-C17-C16         11.94(4)         120.361         120.246           C14-C13         120.4(4)         120.261         120.561           C14-C14         120.3(4)         122.972         122.646           C14-C14-C11         115.4(4) <td< td=""><td></td><td>1.379(5)</td><td></td><td></td></td<>		1.379(5)		
$\begin{array}{ccccccc} C:C2 & 1.361(5) & 1.398 & 1.391 \\ C12C15 & 1.408(5) & 1.372 & 1.365 \\ C2C1 & 1.375(5) & 1.372 & 1.365 \\ \hline \\ $	C4-C3	1.362(5)	1.396	1.389
C12-C15         1.406[5]         1.422         1.416           C15-C16         1.354(5)         1.372         1.365           C2-C1         1.375[5]         1.394         1.388           Table 3.Sperimental and calculated ond angles (") for TMQ.           Atoms         Calculated (B3LYP/6-31 ++G(2d,p))           Calculated (B3LYP/6-31 ++G(2d,p)) <td>C3-C2</td> <td></td> <td>1.398</td> <td>1.391</td>	C3-C2		1.398	1.391
C15-C16 $1.374(5)$ $1.372$ $1.365$ C2-C1 $1.375(5)$ $1.394$ $1.388$ C2-C1Calculated (B3LYP/6-31 ++6(d.p))Calculated (B3LYP/6-31 ++6(d.p))C	C12-C15	1.408(5)		1.416
C2-C1         1.375(5)         1.394         1.388           Table 3. Stperimental and calculated bond angles (*) for TMQ.         Calculated (B31.VP/6-31 ++G(d,p))         Calculated (B31.VP/6-31 ++G(d,p))           C17.02.C19         116.63         118.491         118.275           C11.N4-C12         117.5(4)         120.009         120.134           C7-N1-C6         119.1(4)         120.009         120.134           C7-N1-C6         129.4(4)         128.243         128.271           C8-N2-N1         104.0(3)         105.004         105.087           C2-C17-C16         114.4(4)         114.486         114.519           C14-C17-C16         119.9(4)         120.391         120.288           C17-C18-C13         119.9(4)         120.063         120.041           C14-C13-C12         120.3(4)         120.064         120.296           C14-C13-C13         120.8(4)         120.064         120.296           C14-C13-C13         120.8(4)         120.246         120.296           C14-C10-C11         116.3(3)         113.281         113.494           C7-N3-C9         123.2(4)         122.496         122.555           C14-C10-C11         116.3(3)         113.281         120.6(4)	C15-C16	1.354(5)	1.372	1.365
Table 3. Experimental and calculated bond angles (°) for TMQ.           Atoms         Experimental         Calculated (B3LYP/6-31 ++6(d.p))         Calculated (B3LYP/6-31 ++6(d.p))           C17-02-C19         116.8(3)         118.491         118.275         118.630           C17-02-C19         116.3(3)         118.455         118.630           N2-N1-C6         119.1(4)         120.009         120.134           C7-N1-N2         111.3(3)         111.745         111.594           C7-N1-C6         129.4(4)         128.243         128.271           C6-N2-N1         104.0(3)         105.004         105.087           O2-C17-C16         114.4(4)         114.486         114.519           C18-C17-C16         119.9(4)         120.391         120.288           C17-C16.11         119.9(4)         120.965         119.611           C18-C12         120.3(4)         122.096         124.461           C14-C13-C12         117.4(4)         116.966         116.990           C14-C16-C11         116.3(3)         113.281         13.444           C7-N3         128.1(4)         122.496         122.496           C14-C10-C9         123.2(4)         123.657         130.712           C14-C10				
AtomsExperimentalCalculated (B3LVP/6-31 ++G(d,p))Calculated (B3LVP/6-311 ++G(2d,p))C17-02-C19115.68(3)118.491118.275C17-02-C12117.5(4)118.555118.630N2-N1-C6119.1(4)120.009120.134C7-N1-C6129.4(4)128.243128.271C8-N2-N1104.0(3)105.004105.087O2-C17-C16114.4(4)114.486114.519C17-C18-C16119.9(4)120.391120.288C17-C18-C13119.9(4)120.391120.288C17-C18-C13119.9(4)120.063120.041C14-C13-C12120.3(4)120.063120.041C14-C13-C12117.4(4)116.966116.990C14-C13-C12117.4(4)116.966116.990C14-C10-C9120.5(4)120.246120.289C14-C10-C11116.3(3)113.281113.484C14-C10-C3123.2(4)123.724123.657N3-C9123.2(4)123.724123.657N3-C9123.2(4)123.724123.657N3-C9123.2(4)123.724123.657N3-C9123.2(4)123.724123.657N3-C9123.2(4)123.724123.657N3-C9123.2(4)123.65513.0712O1-C7-N1128.6(4)130.05513.0712O1-C7-N1128.6(4)130.335103.000C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)119.215119.276C3-C4-C4 <th></th> <th></th> <th></th> <th></th>				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Table 3. Experimental and cal	culated bond angles (°) for TMQ.		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Atoms	Experimental	Calculated (B3LYP/6-31 ++G(d.p))	Calculated (B3LYP/6-311 ++G(2d.p))
C11-M-C12       17,5(4)       118,55       118,630         N2-N1-C6       119,1(4)       120,090       120,134         C7-N1-N2       111,3(3)       111,745       111,594         C7-N1-C6       129,4(4)       128,243       128,271         C3-N2-C1       104,0(3)       105,004       105,007         O2-C17-C16       114,4(4)       114,486       114,519         C17-C18-C1       119,9(4)       120,391       120,288         C17-C18-C1       129,9(4)       120,063       120,041         C14-C13-C12       120,3(4)       120,063       120,041         C14-C13-C12       117,4(4)       116,966       116,990         C14-C13-C12       120,5(4)       120,246       120,248         C14-C10-C1       160,3(4)       116,026       16,051         C14-C10-C2       123,2(4)       123,274       123,657         C14-C10-C3       123,0(4)       120,246       120,248         C14-C10-C3       123,0(4)       120,246       120,248         C14-C10-C3       123,0(4)       120,246       120,248         C14-C10-C3       123,0(4)       120,255       120,555         C4-N3-C9       123,0(4)       120,755 <t< td=""><td></td><td><u> </u></td><td></td><td></td></t<>		<u> </u>		
N2-N1-C6191 [4]120.009120.134C7-N1-C6129.4(4)128.243128.271C8-N2-N1104.0(3)105.004105.007C2-L7-C16125.6(4)125.123125.192C2-L7-C16114.4(4)114.486114.519C18-C17-C16119.9(4)120.391120.288C17-C18-C13119.9(4)120.053120.041C18-C17-C16119.9(4)120.053120.041C14-C13-C18122.3(4)122.972122.968C14-C13-C18122.3(4)120.046120.059C14-C13-C18123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)127.72129.630C14-C10-C9123.2(4)120.726123.61C14-C10-C9123.2(4)120.726123.63C7-N3128.1(4)126.309126.286C3-C4-C5120.6(4)120.736120.797C5-C6-C1120.1(4)120.736120.169C1-C5-C4119.2(4)119.151119.622C3-C4-C5120.6(4)120.726121.005C3-C4-C5120.6(4)120.726				
C7-N1-N21113(3)11174511594C7-N1-C61294(4)128243128.271C8-N2-N1104.0(3)105.004105.087C2-C17-C16114.4(4)114.486114.519C3-C17-C16119.9(4)120.391120.288C17-C18-C13119.9(4)129.49120.063120.041C18-C13-C12120.3(4)120.063120.041C14-C13-C12120.3(4)120.063120.041C14-C13-C1217.4(4)116.966116.990C14-C13-C12120.8(4)121.064120.060C14-C13-C12120.8(4)120.246120.289C14-C10-C1116.3(4)116.026116.051C14-C10-C29123.2(4)123.724123.657C14-C10-C3123.0(4)122.90129.630C14-C10-C3123.0(4)122.9702129.630C4-N3-C9123.0(4)122.9702129.630C4-N3-C9123.0(4)120.736120.169C4-N3-C7107.8(4)100.655130.712C4-N3-C7107.8(4)130.655103.000C5-C6-C1120.1(4)120.352120.169C3-C4-C5120.6(4)120.736120.169C3-C4-C5120.6(4)120.262120.169C3-C4-C5120.6(4)120.736120.05C3-C4-C5120.6(4)120.736121.005C3-C4-C5120.6(4)120.736120.05C3-C4-C5120.6(4)120.732123.04C3-C4-C5120.6(4)119.15 <td></td> <td></td> <td></td> <td></td>				
C7-N1-C6       1294(4)       128243       128271         C8-N2-N1       104.0(3)       105.004       105.007         C9-C17-C16       114.4(4)       114.486       114.519         C17-C18-C13       119.9(4)       120.391       120.228         C17-C18-C13       119.9(4)       120.391       120.228         C17-C18-C13       119.9(4)       120.391       120.228         C17-C18-C13       129.3(4)       120.0663       120.041         C14-C13-C18       122.3(4)       122.972       122.968         C14-C13-C18       122.3(4)       120.046       120.060         C14-C13-C18       122.8(4)       121.064       120.600         C14-C10-C11       16.3(5)       113.613       113.844         C14-C10-C11       16.3(6)       116.9051       124.555         C14-C10-C11       16.3(6)       112.0246       120.286         C14-C10-C11       16.3(6)       113.63       13.844         C7-N3       123.0(4)       122.972       129.630         C4N3-C7       107.8(4)       107.074       107.8(1         O1-C7-N1       128.6(4)       107.365       130.010         O1-C7-N1       128.6(4)       120.52 <td< td=""><td></td><td></td><td></td><td></td></td<>				
C8-N2-N1         104.0 <sup>(2)</sup> 105.004         105.087           02-C17-C18         125.6(4)         125.123         125.192           02-C17-C16         114.4(4)         114.486         114.519           C18-C17-C16         119.9(4)         120.2391         120.288           C17-C18-C13         119.9(4)         120.545         119.611           C18-C13-C12         120.3(4)         120.063         120.041           C14-C13-C12         117.4(4)         116.966         116.990           C14-C13-C12         117.4(4)         116.056         116.051           C14-C10-C11         116.3(4)         116.026         116.051           C14-C10-C9         123.2(4)         123.724         123.657           C14-C10-C9         123.2(4)         122.9702         129.630           C4-N3-C9         123.0(4)         122.496         122.555           C8-N3-C7         107.8(4)         107.794         107.803           O1-C7-N3         128.1(4)         126.309         126.286           O1-C7-N3         128.1(4)         120.630         120.049           C3-C4-C1         120.1(4)         120.352         120.169           C1-C-N1         120.6(4)         120.05				
02-C17-C18         125.123         125.192           02-C17-C16         114.4(4)         114.486         114.519           02-C17-C16         119.9(4)         120.391         120.208           C17-C18-C13         119.9(4)         119.545         119.611           C18-C13-C18         122.3(4)         122.972         122.968           C14-C13-C12         117.4(4)         116.966         116.990           C14-C13-C12         117.4(4)         116.966         116.990           C14-C13-C12         117.4(4)         116.966         116.990           C14-C13-C11         116.3(4)         116.026         116.051           C14-C10-C9         123.2(4)         123.724         123.657           N3-GP-C10         113.6(3)         113.281         113.484           C7-N3-C9         123.0(4)         122.496         122.555           C8-N3-C7         107.8(4)         107.794         107.803           O1-C7-N1         128.6(4)         120.355         130.712           O1-C7-N1         128.6(4)         120.55         120.69           O1-C7-N1         128.6(4)         120.56         120.69           O1-C7-N1         128.6(4)         120.57         120.164				
02-C17-C16         114.4 <sup>7</sup> (4)         114.46         114.519           C18-C17-C16         119.9(4)         120.391         120.288           C17-C18-C13         119.9(4)         120.063         120.041           C18-C13-C12         120.3(4)         120.063         120.041           C14-C13-C12         117.4(4)         116.966         116.990           C10-C14-C13         120.8(4)         121.064         120.289           C14-C10-C1         116.3(4)         116.026         116.051           C14-C10-C9         123.2(4)         123.724         123.657           C14-C10-C9         123.0(4)         122.496         122.555           C8-N3-C9         123.0(4)         122.496         122.555           C8-N3-C7         107.8(4)         107.794         107.803           O1-C7-N3         128.1(4)         126.309         126.286           N3-C7-N1         128.6(4)         130.355         130.712           O1-C7-N3         128.1(4)         120.352         120.169           C1-C-K-N1         120.6(4)         120.055         120.169           C1-C-K-N1         120.6(4)         120.05         120.169           C1-C-K-N1         120.1(4)         120.352<	C7-N1-C6	129.4(4)	128.243	128.271
C18-C17-C16         119.9(4)         120.391         120.288           C17-C18-C13         119.9(4)         119.545         119.611           C14-C13-C12         120.3(4)         120.063         120.041           C14-C13-C12         127.3(4)         122.972         122.968           C14-C13-C12         17.4(4)         116.666         116.690           C10-C14-C13         120.8(4)         121.064         121.060           C14-C10-C9         120.5(4)         120.246         120.289           C14-C10-C11         116.3(4)         116.026         116.051           C11-C10-C9         123.2(4)         123.724         123.657           N3-G9-C10         113.6(3)         113.281         113.484           C7-N3-C9         123.0(4)         122.496         122.555           C8-N3-C7         107.8(4)         177.94         107.803           O1-C7-N1         128.6(4)         130.655         130.712           O1-C7-N3         128.1(4)         120.305         130.000           C5-C6-C1         120.1(4)         120.736         120.797           C5-C6-C1         120.1(4)         120.736         120.797           C5-C6-C1         120.6(4)         120.26	C7-N1-C6 C8-N2-N1	129.4(4) 104.0(3)	128.243 105.004	128.271 105.087
C17-C18-C13119.9(4)119.545119.611C18-C13-C12120.3(4)120.063120.041C14-C13-C18122.3(4)122.972122.968C14-C13-C12117.4(4)116.966116.990C10-C14-C13120.8(4)121.064120.289C14-C10-C9120.5(4)120.246120.289C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)123.724123.657C14-C10-C9123.2(4)127.42123.657C8-N3-C9123.0(4)122.496122.555C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.803O1-C7-N3128.1(4)126.309126.286C9-C4-C5120.6(4)120.352120.169C1-C6-N1119.3(4)119.033162.266C3-C4-C5120.6(4)120.552120.169C3-C4-C5120.6(4)120.352120.169C3-C4-C5120.6(4)120.263120.979C5-C6-C1120.3(4)119.213119.217C4-C5120.6(4)120.43119.217C4-C5120.6(4)120.43119.217C4-C1-C1120.0(4)125.470118.915C1-C1-C1118.6(4)118.915118.27V+C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C16-C15-C12120.6(4)120.273120.279C15-C12-C13118.0(4)118.936118.904	C7-N1-C6 C8-N2-N1 O2-C17-C18	129.4(4) 104.0(3) 125.6(4)	128.243 105.004 125.123	128.271 105.087 125.192
CH8-C13-C12         120.3(4)         120.063         120.041           C14-C13-C18         122.3(4)         122.972         122.968           C14-C13-C12         17.4(4)         116.966         116.990           C10-C14-C13         120.8(4)         121.064         120.289           C14-C10-C9         120.5(4)         120.246         120.289           C14-C10-C9         123.2(4)         123.724         123.657           N3-C9-C10         13.6(3)         113.281         113.484           C7-N3-C9         123.0(4)         122.496         122.555           C8-N3-C7         10.78(4)         107.794         107.803           O1-C7-N1         128.6(4)         130.655         130.712           O1-C7-N1         128.1(4)         126.309         126.286           N3-C7-1         10.78(4)         103.035         103.000           C5-C6-C1         120.1(4)         120.352         120.169           C1-C-N1         120.6(4)         120.352         120.169           C1-C6-N1         120.1(4)         120.352         120.169           C1-C6-N1         120.1(4)         120.352         120.169           C1-C6-N1         120.1(4)         120.352         <	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16	129.4(4) 104.0(3) 125.6(4) 114.4(4)	128.243 105.004 125.123 114.486	128.271 105.087 125.192 114.519
C14-C13-C18       122.3(4)       122.972       122.968         C14-C13-C12       117.4(4)       116.966       116.990         C14-C13-C12       120.5(4)       121.064       121.060         C14-C10-C9       120.5(4)       120.246       120.289         C14-C10-C11       116.3(3)       113.281       113.484         C7-N3-C9       123.0(4)       122.496       122.555         C8-N3-C7       107.8(4)       107.794       107.803         O1-C7-N1       128.6(4)       130.635       130.010         O1-C7-N1       128.6(4)       130.635       130.010         O1-C7-N3       128.1(4)       120.352       120.169         O1-C7-N1       128.6(4)       130.335       130.000         C5-C6-N1       120.1(4)       120.352       120.169         C1-C6-N1       119.3(4)       119.912       119.033         C5-C6-C1       120.6(4)       121.026       120.05         C3-C4-C5       120.6(4)       121.026       120.05         C3-C4-C5       120.6(4)       120.22       120.61         C4-C5-C4       119.2(4)       119.152       119.03         C4-C5-C5       120.6(4)       120.27       120.570	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C18-C17-C16	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4)	128.243 105.004 125.123 114.486 120.391	128.271 105.087 125.192 114.519 120.288
C14-C13-C12       117.4(1)       116.966       116.990         C10-C14-C13       120.8(4)       121.064       121.060         C14-C10-C9       120.5(4)       120.246       120.289         C14-C10-C11       116.3(4)       116.026       116.051         C11-C10-C9       123.2(4)       123.724       123.657         N3-C9-C10       113.6(3)       113.281       113.484         C7-N3-C9       123.0(4)       122.496       122.555         C8-N3-C7       107.8(4)       107.794       107.803         O1-C7-N1       128.6(4)       130.655       130.712         O1-C7-N3       128.1(4)       120.305       103.000         C5-C6-C1       120.1(4)       120.325       120.169         C1-C6-N1       119.3(4)       118.912       119.033         C6-C5-C4       120.6(4)       120.26       120.05         C3-C4-C5       120.6(4)       120.126       120.105         C3-C4-C5       120.6(4)       120.32       129.121         N4-C11-C10       115.4(4)       115.611       115.700         N4-C11-C10       126.0(4)       125.473       125.470         C1-C4-S1       120.6(4)       125.473       125.470<	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C18-C17-C16 C17-C18-C13	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 119.9(4)	128.243 105.004 125.123 114.486 120.391 119.545	128.271 105.087 125.192 114.519 120.288 119.611
C10-C14-C13120.8(4)121.064121.060C14-C10-C9120.5(4)120.246120.289C14-C10-C11116.3(4)116.026116.051C11-C10-C9123.2(4)123.724123.657N3-C9-C10113.6(3)113.281113.484C7-N3-C9123.0(4)122.496122.555C8-N3-C7107.8(4)107.794107.803O1-C7-N1128.6(4)130.655130.712O1-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.352120.169C1-C6-N1119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C11118.4(4)118.915118.827N4-C12-C13120.0(4)125.473125.470C10-C11-C11118.6(4)118.915118.827N4-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)120.792120.874N2-C8-N3113.5(4)112.072120.874N2-C8-N3113.5(4)112.072120.874N2-C8-N3113.5(4)120.792 <td< td=""><td>C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12</td><td>129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 119.9(4) 120.3(4)</td><td>128.243 105.004 125.123 114.486 120.391 119.545 120.063</td><td>128.271 105.087 125.192 114.519 120.288 119.611 120.041</td></td<>	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 119.9(4) 120.3(4)	128.243 105.004 125.123 114.486 120.391 119.545 120.063	128.271 105.087 125.192 114.519 120.288 119.611 120.041
C14-C10-C1120.5(4)120.246120.289C14-C10-C11116.3(4)116.026116.051C14-C10-C11116.3(4)123.724123.657N3-C9-C10113.6(3)113.281113.484C7-N3-C9123.0(4)122.496122.555C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.80301-C7-N1128.6(4)130.655130.71201-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-C1120.6(4)120.736120.797C5-C6-C1120.6(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C11115.4(4)115.611115.700N4-C11-C11118.6(4)118.915118.827N4-C12-C13119.9(4)119.152119.304C15-C12120.6(4)120.728120.794C15-C12120.6(4)120.792120.874N4-C12-C13118.0(4)118.916118.904C16-C15-C12120.6(4)120.792120.874N2-C8-N3113.5(4)120.728120.711	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 119.9(4) 120.3(4) 122.3(4)	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968
C14-C10-C11       116.3(4)       116.026       116.051         C11-C10-C9       123.2(4)       123.724       123.657         N3-C9-C10       113.6(3)       113.281       113.484         C7-N3-C9       123.0(4)       122.496       122.555         C8-N3-C7       129.2(4)       129.702       129.630         C8-N3-C7       128.6(4)       130.655       130.712         01-C7-N1       128.6(4)       126.309       126.286         N3-C7-N1       128.1(4)       120.303       103.000         C5-C6-N1       120.6(4)       120.736       120.797         C5-C6-C1       120.1(4)       120.352       120.169         C1-C6-N1       19.3(4)       18.912       119.033         C6-C5-C4       120.2(4)       121.026       120.05         C3-C4-C5       120.6(4)       121.026       121.005         C2-C3-C4       120.3(4)       125.473       125.470         C10-C11-C11       115.4(4)       115.611       115.700         N4-C11-C10       126.0(4)       125.473       125.470         C10-C11-C11       118.6(4)       118.915       118.827         N4-C12-C15       119.9(4)       119.152       12.304 <td>C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12</td> <td>129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 120.3(4) 122.3(4) 117.4(4)</td> <td>128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966</td> <td>128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990</td>	C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 120.3(4) 122.3(4) 117.4(4)	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990
C11-C10-C9123.2(4)123.724123.657N3-C9-C10113.6(3)113.281113.484C7-N3-C9123.0(4)122.496122.555C8-N3-C7107.8(4)107.794107.803O1-C7-N1128.6(4)130.655130.712O1-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.2(4)119.512119.033C6-C5-C4120.3(4)119.213119.217C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C11118.6(4)118.915118.827N4-C12-C13122.1(4)121.912121.791N4-C12-C13118.0(4)118.915118.827N4-C12-C13118.0(4)118.936118.904C16-C5-C12120.6(4)120.273120.279C15-C12-C13118.0(4)18.936118.904C16-C5-C12120.6(4)120.273120.279C15-C12-C13113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12	129.4(4) 104.0(3) 125.6(4) 114.4(4) 119.9(4) 120.3(4) 122.3(4) 117.4(4)	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990
N3-C9-C10113.6(3)113.281113.484C7-N3-C9123.0(4)122.496122.555C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.80301-C7-N1128.6(4)130.655130.71201-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C10126.0(4)125.473125.470C10-C11-C11118.6(4)118.915118.827N4-C12-C13122.1(4)121.912121.912N4-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C16-C15-C12120.6(4)120.273120.279C15-C16-C17121.1(4)120.792120.874N2-C8-N313.5(4)120.728120.711	C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C10-C14-C13	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $117.4(4)$ $120.8(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060
C7-N3-C9123.0(4)122.496122.555C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.80301-C7-N1128.6(4)130.655130.71201-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C1115.4(4)115.611115.700N4-C11-C10126.0(4)121.921121.791N4-C12-C13122.1(4)121.912121.791N4-C12-C13119.9(4)119.152119.304C15-C12-C13118.0(4)118.936118.904C15-C12-C13120.6(4)120.273120.279C15-C12-C13120.6(4)120.273120.279C15-C12-C13120.6(4)120.273120.874N2-C8-N313.5(4)120.728120.711	C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C18 C14-C13-C12 C10-C14-C13 C14-C10-C9	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $117.4(4)$ $120.8(4)$ $120.5(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060 120.289
C7-N3-C9123.0(4)122.496122.555C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.80301-C7-N1128.6(4)130.655130.71201-C7-N3128.1(4)126.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N119.3(4)118.912119.033C6-C5-C4120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C1115.4(4)115.611115.700N4-C11-C10126.0(4)121.912121.791N4-C12-C13122.1(4)121.912121.791N4-C12-C13118.0(4)118.915118.827N4-C12-C13119.9(4)119.152119.304C15-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C15-C12-C13120.6(4)120.273120.279C15-C12-C13120.6(4)120.273120.874N2-C8-N313.5(4)120.728120.711	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C10-C14-C13 C14-C10-C9 C14-C10-C11	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $117.4(4)$ $120.8(4)$ $120.5(4)$ $116.3(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060 120.289 116.051
C8-N3-C9129.2(4)129.702129.630C8-N3-C7107.8(4)107.794107.80301-C7-N1128.6(4)130.655130.71201-C7-N3128.1(4)26.309126.286N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C10126.0(4)125.473125.470C10-C11-C11118.6(4)118.915118.827N4-C12-C13122.1(4)121.912121.791N4-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)120.273120.279C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417125.12C3-C2-C1119.9(4)120.728120.711	C7-N1-C6 C8-N2-N1 O2-C17-C18 C17-C16 C17-C16-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C10-C14-C13 C14-C10-C9 C14-C10-C11 C11-C10-C9	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $120.8(4)$ $120.5(4)$ $116.3(4)$ $123.2(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060 120.289 116.051 123.657
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N3-C7-N1103.4(4)103.035103.000C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C11115.4(4)118.915118.827N4-C11-C11118.6(4)118.915118.827N4-C12-C13122.1(4)121.912121.791N4-C12-C15119.9(4)119.152119.304C15-C12-C13118.0(4)118.936118.904C15-C12-C13118.0(4)120.792120.874C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	C7-N1-C6 C8-N2-N1 02-C17-C18 02-C17-C16 C18-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C14-C13-C12 C14-C10-C9 C14-C10-C9 N3-C9-C10 C7-N3-C9 C8-N3-C9 C8-N3-C7	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $116.3(4)$ $123.2(4)$ $113.6(3)$ $123.0(4)$ $129.2(4)$ $107.8(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$
C5-C6-N1120.6(4)120.736120.797C5-C6-C1120.1(4)120.352120.169C1-C6-N1119.3(4)118.912119.033C6-C5-C4119.2(4)119.151119.262C3-C4-C5120.6(4)121.026121.005C2-C3-C4120.3(4)119.213119.217N4-C11-C11115.4(4)115.611115.700N4-C11-C10126.0(4)125.473125.470C10-C11-C11118.6(4)118.915118.827N4-C12-C13122.1(4)121.912121.791N4-C12-C15119.9(4)119.152119.304C15-C12-C13118.0(4)118.936118.904C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C17-C16-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C14-C13-C12 C14-C10-C9 C14-C10-C9 C14-C10-C9 N3-C9-C10 C7-N3-C9 C8-N3-C7 O1-C7-N1	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $120.8(4)$ $120.5(4)$ $116.3(4)$ $123.2(4)$ $113.6(3)$ $123.0(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7-N1-C6 C8-N2-N1 O2-C17-C18 O2-C17-C16 C17-C18-C13 C18-C13-C12 C14-C13-C12 C14-C13-C12 C14-C13-C12 C14-C10-C9 C14-C10-C9 N3-C9-C10 C7-N3-C9 C8-N3-C9 C8-N3-C7 O1-C7-N1 O1-C7-N1 O1-C7-N1 C5-C6-C1	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $116.3(4)$ $123.2(4)$ $113.6(3)$ $123.0(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$ $128.1(4)$ $103.4(4)$ $120.6(4)$ $120.1(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.736 120.352	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$
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N4-C12-C15119.9(4)119.152119.304C15-C12-C13118.0(4)118.936118.904C16-C15-C12120.6(4)120.273120.279C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C10-C14-C13} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C3-N3-C9} \\ \text{C8-N3-C7} \\ \text{C6-N3-C9} \\ \text{C8-N3-C7} \\ \text{O1-C7-N1} \\ \text{O1-C7-N3} \\ \text{N3-C7-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C3-C3-C4} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C11} \\ \text{N4-C11-C11} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $128.6(4)$ $128.1(4)$ $103.4(4)$ $120.6(4)$ $120.1(4)$ $119.2(4)$ $120.6(4)$ $120.6(4)$ $120.3(4)$ $125.4(4)$ $126.0(4)$	128.243 $105.004$ $125.123$ $114.486$ $120.391$ $119.545$ $120.063$ $122.972$ $116.966$ $121.064$ $120.246$ $116.026$ $123.724$ $113.281$ $122.496$ $129.702$ $107.794$ $130.655$ $126.309$ $103.035$ $120.736$ $120.352$ $118.912$ $119.151$ $121.026$ $119.213$ $115.611$ $125.473$	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$
C15-C12-C13118.0(4)118.936118.904C16-C15-C12120.6(4)120.273120.279C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C10-C14-C13} \\ \text{C14-C10-C9} \\ \text{C14-C10-C10} \\ \text{C10-C11-C11} \\ \textbf{C10-C11-C11} \\ \textbf{C10-C11-C11-C11} \\ \textbf{C10-C11-C11-C11} \\ \textbf{C10-C11-C11-C11} \\ \textbf{C10-C11-C11} \\$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.0(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$ $128.1(4)$ $103.4(4)$ $120.6(4)$ $120.1(4)$ $119.2(4)$ $120.6(4)$ $120.3(4)$ $125.4(4)$ $126.6(4)$ $120.3(4)$ $115.4(4)$ $126.0(4)$ $118.6(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.736 120.352 118.912 119.151 121.026 119.213 115.611 125.473 118.915	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$
C16-C15-C12120.6(4)120.273120.279C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C10-C14-C13} \\ \text{C14-C10-C9} \\ \text{C3-C3-C10} \\ \text{C7-N3-C9} \\ \text{C8-N3-C7} \\ \text{C3-C4-C5} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C11} \\ \text{N4-C11-C10} \\ \text{C10-C11-C11} \\ \text{N4-C12-C13} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $124.4(4)$ $120.6(4)$ $120.6(4)$ $120.3(4)$ $125.4(4)$ $126.6(4)$ $120.3(4)$ $115.4(4)$ $126.6(4)$ $126.0(4)$ $118.6(4)$ $122.1(4)$	128.243 $105.004$ $125.123$ $114.486$ $120.391$ $119.545$ $120.063$ $122.972$ $116.966$ $121.064$ $120.246$ $116.026$ $123.724$ $113.281$ $122.496$ $129.702$ $107.794$ $130.655$ $126.309$ $103.035$ $120.736$ $120.736$ $120.736$ $120.736$ $120.352$ $118.912$ $119.151$ $121.026$ $119.213$ $118.915$ $121.912$	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$ $121.791$
C15-C16-C17121.1(4)120.792120.874N2-C8-N3113.5(4)112.417112.512C3-C2-C1119.9(4)120.728120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C11} \\ \text{C11-C10-C9} \\ \text{N3-C9-C10} \\ \text{C7-N3-C9} \\ \text{C8-N3-C9} \\ C$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $116.3(4)$ $123.2(4)$ $113.6(3)$ $123.0(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$ $128.6(4)$ $128.6(4)$ $120.1(4)$ $119.3(4)$ $119.2(4)$ $120.6(4)$ $120.3(4)$ $115.4(4)$ $126.0(4)$ $118.6(4)$ $122.1(4)$ $119.9(4)$	128.243 $105.004$ $125.123$ $114.486$ $120.391$ $119.545$ $120.063$ $122.972$ $116.966$ $121.064$ $120.246$ $116.026$ $123.724$ $113.281$ $122.496$ $129.702$ $107.794$ $130.655$ $126.309$ $103.035$ $120.736$ $120.352$ $118.912$ $119.151$ $121.026$ $119.213$ $115.611$ $125.473$ $118.915$ $121.912$ $119.152$	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$ $121.791$ $119.304$
N2-C8-N3 113.5(4) 112.417 112.512 C3-C2-C1 119.9(4) 120.728 120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C11} \\ \text{C11-C10-C9} \\ \text{N3-C9-C10} \\ \text{C7-N3-C9} \\ \text{C8-N3-C9} \\ \text{C8-N3-C9} \\ \text{C8-N3-C7} \\ \text{O1-C7-N1} \\ \text{O1-C7-N1} \\ \text{O1-C7-N3} \\ \text{N3-C7-N1} \\ \text{C5-C6-N1} \\ \text{C5-C6-N1} \\ \text{C5-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C5-C4} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C11} \\ \text{N4-C11-C10} \\ \text{C10-C11-C11} \\ \text{N4-C12-C13} \\ \text{N4-C12-C15} \\ \text{C15-C12-C13} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $120.6(4)$ $120.1(4)$ $119.3(4)$ $120.6(4)$ $120.3(4)$ $115.4(4)$ $126.0(4)$ $126.0(4)$ $122.1(4)$ $119.9(4)$ $118.0(4)$	128.243 $105.004$ $125.123$ $114.486$ $120.391$ $119.545$ $120.063$ $122.972$ $116.966$ $121.064$ $120.246$ $116.026$ $123.724$ $113.281$ $122.496$ $129.702$ $107.794$ $130.655$ $126.309$ $103.035$ $120.336$ $120.352$ $118.912$ $119.151$ $121.026$ $119.213$ $115.611$ $125.473$ $118.915$ $121.912$ $119.152$ $118.936$	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$ $121.791$ $119.304$
C3-C2-C1 119.9(4) 120.728 120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C11} \\ \text{C11-C10-C9} \\ \text{N3-C9-C10} \\ \text{C7-N3-C9} \\ \text{C8-N3-C9} \\ \text{C8-N3-C7} \\ \text{O1-C7-N1} \\ \text{O1-C7-N3} \\ \text{N3-C7-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C6-C5-C4} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C11} \\ \text{N4-C12-C13} \\ \text{N4-C12-C13} \\ \text{N4-C12-C13} \\ \text{C15-C12-C13} \\ \text{C16-C15-C12} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $120.6(4)$ $120.1(4)$ $119.3(4)$ $120.6(4)$ $120.3(4)$ $115.4(4)$ $126.0(4)$ $126.0(4)$ $122.1(4)$ $119.9(4)$ $118.0(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.352 118.912 119.151 121.026 119.213 115.611 125.473 118.915 121.912 118.936 120.273	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060 120.289 116.051 123.657 113.484 122.555 129.630 107.803 130.712 126.286 103.000 120.797 120.169 119.033 119.262 121.005 119.217 115.700 125.470 118.827 121.791 119.304 118.904 120.279
C3-C2-C1 119.9(4) 120.728 120.711	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C14-C10-C9} \\ \text{C14-C10-C11} \\ \text{C11-C10-C9} \\ \text{N3-C9-C10} \\ \text{C7-N3-C9} \\ \text{C8-N3-C9} \\ \text{C8-N3-C7} \\ \text{O1-C7-N1} \\ \text{O1-C7-N3} \\ \text{N3-C7-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C6-C5-C4} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C11} \\ \text{N4-C12-C13} \\ \text{N4-C12-C13} \\ \text{N4-C12-C13} \\ \text{C15-C12-C13} \\ \text{C16-C15-C12} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$ $128.1(4)$ $103.4(4)$ $120.6(4)$ $120.6(4)$ $120.6(4)$ $122.1(4)$ $118.6(4)$ $122.1(4)$ $119.9(4)$ $128.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.352 118.912 119.151 121.026 119.213 115.611 125.473 118.915 121.912 118.936 120.273	128.271 105.087 125.192 114.519 120.288 119.611 120.041 122.968 116.990 121.060 120.289 116.051 123.657 113.484 122.555 129.630 107.803 130.712 126.286 103.000 120.797 120.169 119.033 119.262 121.005 119.217 115.700 125.470 118.827 121.791 119.304 118.904 120.279
	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C7-N3-C9} \\ \text{C8-N3-C7} \\ \text{C0-C10} \\ \text{C7-N3} \\ \text{C1-C7-N1} \\ \text{O1-C7-N3} \\ \text{N3-C7-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C5-C6-C1} \\ \text{C1-C6-N1} \\ \text{C6-C5-C4} \\ \text{C3-C4-C5} \\ \text{C2-C3-C4} \\ \text{N4-C11-C10} \\ \text{C10-C11-C11} \\ \text{N4-C12-C13} \\ \text{C15-C12-C13} \\ \text{C16-C15-C12} \\ \text{C15-C12-C13} \\ \text{C15-C16-C17} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $120.5(4)$ $120.5(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.0(4)$ $129.2(4)$ $107.8(4)$ $128.6(4)$ $128.1(4)$ $103.4(4)$ $120.6(4)$ $120.6(4)$ $120.3(4)$ $115.4(4)$ $126.0(4)$ $118.6(4)$ $122.1(4)$ $119.9(4)$ $118.0(4)$ $120.6(4)$ $120.6(4)$ $122.1(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.736 120.352 118.912 119.151 121.026 119.213 115.611 125.473 118.915 121.912 118.936 120.273 120.792	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$ $121.791$ $119.304$ $118.904$ $120.279$ $120.874$
	$\begin{array}{c} \text{C7-N1-C6} \\ \text{C8-N2-N1} \\ \text{O2-C17-C18} \\ \text{O2-C17-C16} \\ \text{C18-C17-C16} \\ \text{C17-C18-C13} \\ \text{C18-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C13-C12} \\ \text{C14-C10-C9} \\ \text{C14-C10-C10} \\ \text{C10-C1-C10} \\ \text{C10-C1-C11} \\ \text{N4-C12-C13} \\ \text{C10-C1-C11} \\ \text{N4-C12-C13} \\ \text{C15-C12-C13} \\ \text{C15-C12-C12} \\ \text{C15-C12-C12} \\ \text{C15-C12-C17} \\ \text{N2-C8-N3} \\ \end{array}$	129.4(4) $104.0(3)$ $125.6(4)$ $114.4(4)$ $119.9(4)$ $120.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $122.3(4)$ $122.5(4)$ $116.3(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $123.2(4)$ $124.4(4)$ $124.4(4)$ $120.6(4)$ $120.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$ $122.1(4)$ $119.9(4)$ $120.6(4)$ $121.1(4)$ $113.5(4)$	128.243 105.004 125.123 114.486 120.391 119.545 120.063 122.972 116.966 121.064 120.246 116.026 123.724 113.281 122.496 129.702 107.794 130.655 126.309 103.035 120.736 120.352 118.912 119.151 121.026 119.213 115.611 125.473 118.915 121.912 119.152 118.936 120.273 120.792 112.417	128.271 $105.087$ $125.192$ $114.519$ $120.288$ $119.611$ $120.041$ $122.968$ $116.990$ $121.060$ $120.289$ $116.051$ $123.657$ $113.484$ $122.555$ $129.630$ $107.803$ $130.712$ $126.286$ $103.000$ $120.797$ $120.169$ $119.033$ $119.262$ $121.005$ $119.217$ $115.700$ $125.470$ $118.827$ $121.791$ $119.304$ $118.904$ $120.279$ $120.874$ $112.512$

Table 2. Experimental and calculated bond lengths (Å) for TMQ.

The Cg1: N1/N2/C8/N3/C7 makes dihedral angles of 78.1(2) and 77.54(18)° with Cg3:C1-C6 and Cg5:N4/C11/C10/C14/C13/C18/C17/C16/C15/C12, respectively. The dihedral angle between Cg3 and Cg5 is  $81.31(17)^\circ$ . In the crystal structure (Table 5 and Figure 2), the intermolecular

hydrogen bonds (C(8)-H(8)…O(1)) and intermolecular interaction of the type C(9)-H(9A)[1]  $\rightarrow$  Cg(3) are observed and also intramolecular hydrogen bonds (Table 5) of the type C-H…N and C-H…O are viewed.

Atoms	Experimental	Calculated (B3LYP/6-31 ++G(d,p))	Calculated (B3LYP/6-311 ++G(2d,p))
D2-C17-C18-C13	178.8(3)	-179.74	-179.7641
11-N2-C8-N3	0.7(4)	-0.2628	-0.221
I2-N1-C6-C1	-4.5(5)	0.61318	0.8157
V2-N1-C6-C5	175.5(3)	-179.27	-179.9411
N2-N1-C7-O1	178.6(4)	-179.83	-179.9411
V2-N1-C7-N3	-1.1(4)	0.40339	0.3116
V3-C9-C10-C11	72.1(4)	93.382	93.1891
N3-C9-C10-C14	-108.8(4)	-85.798	-86.4007
V4-C12-C13-C14	-1.1(5)	-0.3902	-0.4741
V4-C12-C13-C18	-179.9(3)	179.709	179.6304
N4-C12-C15-C16	178.7(3)	-179.762	-179.7144
C1-C2-C3-C4	0.4(7)	-0.00438	0.0114
2-C1-C6-N1	-179.6(3)	-179.933	-179.9218
2-C1-C6-C5	0.4(6)	-0.04305	0.0238
2-C3-C4-C5	0.0(7)	0.00853	0.0119
C3-C4-C5-C6	-0.2(6)	-0.02968	-0.0169
24-C5-C6-N1	-180.0(3)	179.935	179.9436
C4-C5-C6-C1	0.0(6)	0.04691	-0.0011
C6-N1-N2-C8	-175.8(3)	179.782	179.8188
C6-N1-C7-O1	-5.9(6)	0.29240	0.1822
C6-N1-C7-N3	174.5(3)	-179.471	-179.5652
C6-C1-C2-C3	-0.6(6)	0.02160	-0.0291
C7-N1-N2-C8	0.2(4)	-0.1035	-0.0694
C7-N1-C6-C1	-179.7(4)	-179.521	-179.3168
C7-N1-C6-C5		0.5886	0.738
	0.3(5)		0.738
C7-N3-C8-N2	-1.4(5) 62.9(4)	0.5289	87.0644
C7-N3-C9-C10		87.4729	
C8-N3-C7-O1	-178.2(4)	179.684	179.8111
C8-N3-C7-N1	1.4(4)	-0.5383	-0.4265
C8-N3-C9-C10	-117.4(4)	-91.375	-92.2879
C9-N3-C7-O1	1.5(6)	0.6145	0.3349
C9-N3-C7-N1	-178.8(3)	-179.607	-179.9026
C9-N3-C8-N2	178.8(3)	179.508	179.8543
C9-C10-C11-Cl1	-1.9(5)	0.62079	0.1931
C9-C10-C11-N4	177.4(4)	179.757	179.8796
C9-C10-C14-C13	-178.2(3)	179.259	179.5551
C11-N4-C12-C13	0.4(5)	-0.08046	-0.0464
C11-N4-C12-C15	-179.3(3)	179.878	179.9016
C11-C10-C14-C13	1.0(5)	0.01812	-0.0649
C12-N4-C11-Cl1	-179.6(3)	-179.792	-179.7365
C12-N4-C11-C10	1.1(6)	0.57460	0.5683
C12-C13-C14-C10	0.3(5)	0.40370	0.5128
C12-C13-C18-C17	0.8(5)	0.07475	0.1291
C12-C15-C16-C17	1.7(6)	0.0285	0.0353
C13-C12-C15-C16	-1.1(5)	0.1977	0.235
C14-C10-C11-Cl1	178.9(3)	179.833	179.7988
C14-C10-C11-N4	-1.8(6)	-0.545	-0.5147
C14-C13-C18-C17	-177.9(3)	-179.819	-179.7598
C15-C12-C13-C14	178.6(3)	179.650	179.5777
C15-C12-C13-C18	-0.2(5)	-0.250	-0.3177
C15-C16-C17-O2	179.8(3)	179.702	179.6871
C15-C16-C17-C18	-1.1(6)	-0.2094	-0.2302
C16-C17-C18-C13	-0.1(5)	0.15403	0.1437
C18-C13-C14-C10	179.1(3)	-179.698	-179.595
C19-02-C17-C16	-172.1(3)	-179.189	-179.1433
C19-02-C17-C18	8.9(5)	0.71771	0.7693

 Table 5. Intermolecular and Intramolecular interactions of TMQ.

D-H···A/Cg	D-H	H…A/Cg	D···A	D-H…A	Symmetry
C(1)-H(1)···N(2)	0.93	2.43	2.767(6)	102	
C(5)-H(5)···O(1)	0.93	2.30	2.934(5)	125	
C(8)-H(8)····O(1)	0.93	2.27	3.180(5)	167	1/2-x, 1/2+y, 1/2-z
$C(9)-H(9A)[1] \rightarrow Cg(3)$		2.68	3.499(4)	143	1+ <i>x</i> , <i>y</i> , <i>z</i>

#### 3.2. Hirshfeld surface calculations

Hirshfeld surface analysis is a graphical tool for visualization and was carried out to comprehend relative contributions of various molecular contacts to intermolecular interactions in TMQ [43]. The Hirshfeld surface is a drawing of shape engaged by a molecule in the crystal structure and can be constructed from the electron division [44,45]. The 2D (two-dimensional) fingerprint plots [46,47] obtained by Hirshfeld surface analysis can classify each type of intermolecular interactions, and their relative input can be obtained from the area of the surfaces. The 2D fingerprint plots are constructed based on  $d_e$  and  $d_i$  distances scales,

displayed on the graph axes, in which the  $d_e$  represents the distance between the Hirshfeld surface and the nearest atom<sub>outside</sub>, while the  $d_i$  represents the distance between this surface and the nearest atom<sub>inside</sub>. The crystal structure packing of the C<sub>19</sub>H<sub>15</sub>N<sub>4</sub>ClO<sub>2</sub>compound was generated and quantified with Hirshfeld surface analysis and the associated 2D-fingerprint plots using Crystal Explorer package [48] which accepts a crystal structure input file in CIF format.

The 2D fingerprint plot for all the intermolecular interacttions are shown in Figure 3. The H…H interactions which show the most significant contribution of 34.6% to the total Hirshfeld surfaces are reflected in the middle of scattered points in the 2D fingerprint plot.

Intercontacts	Contribution (%)	Intercontacts	Contribution (%)	
Н…Н	34.6	С…С	06.0	
С…Н/Н…С	20.0	C···Cl/Cl···C	01.0	
N····H/H····N	12.8	C···N/N···C	02.7	
0H/HO	11.1	CO/OC	00.5	
Cl····H/H····Cl	10.5	Cl0/0Cl	00.8	
	2			

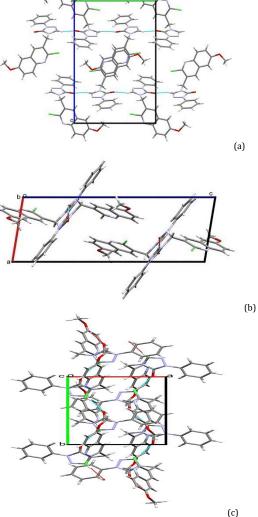


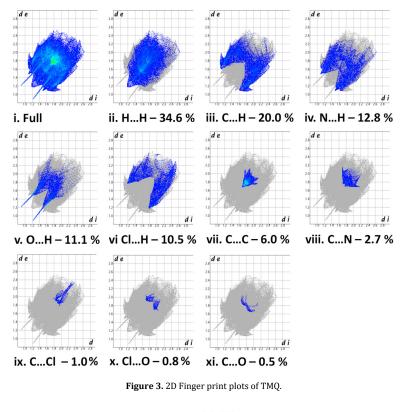
Figure 2. Packing of the molecules viewed along the *a*-(a), *b*-(b) and *c*-axis (c).

The C···H interactions appear as two wings and show a contribution of 20%. The N···H interaction is identified by sharp peaks which comprises 12.8% of the total Hirshfeld surface. The O···H intermolecular contact has covered 11.1% of total Hirshfeld surface area of the molecule apart from that, there are smaller contributions of Cl...H (10.5%), C···C (6.0%), C···Cl (1.0%), C···N (2.7%), C···O (0.5%), and Cl···O (0.8%) (Table 6). Hence, Hirshfeld surface analysis and fingerprint plots illustrate that the crystal lattice is stabilized by four major interactions H···H, C···H, N···H, and O···H.

In the  $d_{norm}$  surface intermolecular contacts relative to the van der Waals radii are represented by method of red-whiteblue color scheme where red regions denote shorter contacts with a negative  $d_{norm}$  value (higher electron density regions), white regions indicate the distance of contacts exactly comparable to the Van der Waals separation with zero  $d_{norm}$  value and blue regions represent longer contacts with a positive  $d_{norm}$  value (lower electron density regions) [49]. The large circular deep red colored depressions visible on  $d_{norm}$  surfaces indicate hydrogen bonding contacts such asC-H···O and additional spots are due to H-H contacts. The intermolecular interactions are also revealed from the views of electro-static potential mapped over Hirshfeld surface, shown in Figure 4. The acceptor and donor atoms participating in these interactions are shown with respective negative (red regions) and positive electrostatic potentials (blue regions).

#### 3.3. DFT Calculations

The potential energy surface (PES) scan has been carried out on dihedral angles  $C_1$ - $C_3$ - $C_{12}$ - $H_{14}$ ,  $C_{30}$ - $N_{35}$ - $C_{12}$ - $H_{14}$  at HF/6-31G level to examine all possible conformations of the title compound. The PES scan was done by minimizing the potential energy in all geometrical parameters by changing the dihedral angle for 360° rotation for both dihedral angles at steps of every 20°.



**Figure 4.** *d<sub>norm</sub>* mapped over the Hirshfeld surface with color scale in the range -0.21 au (red) to 1.2 au (blue), green dotted lines show C-H···O intermolecular interaction. The acceptor and donor atoms are shown with respective negative (red) and positive electrostatic potentials (blue).

The geometry of molecule at local minima is selected on the basis of results obtained in PES scan study. The geometry at local minima has been assumed as starting point for the optimization calculation by utilizing Becke's three parameter hybrid model with the Lee-Yang-Parr correlation functional (B3LYP) method. The geometrical parameters (bond lengths, bond angles and dihedral angles) obtained by B3LYP/6-31++G(d,p) and B3LYP/6-31++G(2d,p) methods are compared with experimental results and were found to be reasonably in good agreement with each other (Tables 1-3).

Eventually the theoretical and experimental values differ slightly, as the experimental values of molecule have been recorded in solid phase while theoretical values were computed in gas phase. The optimized structure (Figure 5) from theoretical calculation (DFT) is superimposed with the molecular skeleton from XRD, giving a molecular overlay RMSD value of 0.09 Å (Figure 6). From the obtained results, it is concluded that the B3LYP calculations very well reproduced the geometry of TMQ.

#### 3.4. Molecular electrostatic potential (MEP)

The MEP plot of TMQ (Figure 5) provides a visual image of the chemically active sites and comparative reactivity of atoms. The negative electrostatic potential (red) regions are mainly localized of C=O and C=N group and are promising sites for electrophilic attack. The positive regions (blue) are localized on all the rings, representing possible sites for nucleophilic attack.

#### 3.5. Frontier molecular orbitals

The frontier molecular orbital, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are key factors for quantum chemistry and the way of the molecule interacts with other species may be analyzed by knowing the HOMO and LUMO energy values. For organic derivatives, the HOMO-LUMO gap is very important because they relate to specific movements of electrons and may be most significant for single electron transfer.

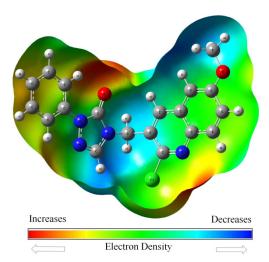


Figure 5. The optimized geometry and MEP plot of TMQ.

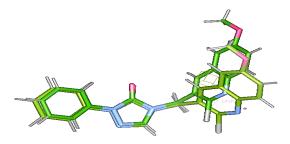


Figure 6. Superimposition diagram TMQ, experimental (Yellow stick model) and theoretical (Green stick model).

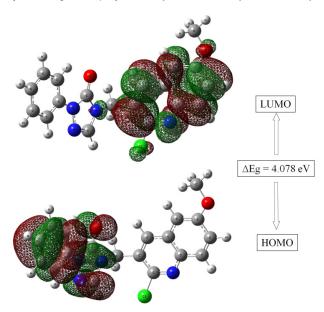


Figure 7. The molecular orbitals and energies for the HOMO and LUMO of TMQ.

The value of HOMO, LUMO and HOMO-LUMO energy gap for the TMQ was calculated by DFT/B3LYP method with 6-311++G(2d,p) basis set. The electron density plots of the HOMO and LUMO for the title molecule is presented in Figure 7. As can be seen from Figure 7 of TMQ, the HOMO is delocalized over the triazole and phenyl ring and LUMO localized over quinoline moiety.The energy values of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of TMQ are about -6.164 and -2.086 eV, respectively. In the present study, calculated  $(Eg = E_{HOMO}-E_{LUMO})$  energy gap is found to be 4.078 eVwhich shows that there is a transfer of electrons from HOMO to LUMO. Accordingly, the HOMO–LUMO transition implied an electron density transfer from the triazole to quinoline.

#### 3.6. Electronic absorption spectra

Figure 8 showed the experimental absorption spectra of the compound TMQ.

Experimenta	l method	TD-DFT B	3LYP/6-311+	++G (2d,p)						
Ethanol	Acetonitrile	Gas			Ethanol			Acetonitr	ile	
۱ (nm) Abs.	λ (nm) Abs.	λ (nm)	E (eV)	f	λ (nm)	E (eV)	f	λ (nm)	E (eV)	f
241	252	343.11	3.6135	0.0026	325.60	3.8079	0.0193	326.87	3.7931	0.0273
327	336	318.73	3.8900	0.0676	322.65	3.8427	0.0731	324.43	3.8216	0.0639
		280.85	4.4146	0.0156	282.94	4.3820	0.0193	284.24	4.3619	0.0196
		272.70	4.5465	0.0046	264.69	4.6842	0.0194	265.91	4.6626	0.0175
		271.24	4.5710	0.0252	261.90	4.7340	0.2104	262.92	4.7156	0.2116
		268.52	4.6173	0.0004	257.35	4.8178	0.1212	258.39	4.7983	0.0977
юмо			-6.3820			-6.3571			-6.1443	
JUMO			-2.1075			-2.0686			-2.0530	
Energy gap			4.2745			4.2885			4.0913	

**Table 7.** Experimental and calculated absorption wavelength  $\lambda$  (nm), excitation energies *E* (eV), and oscillator strengths (*f*) of TMQ calculated by the B3LYP method using 6-311++G(2d,p)basis set.

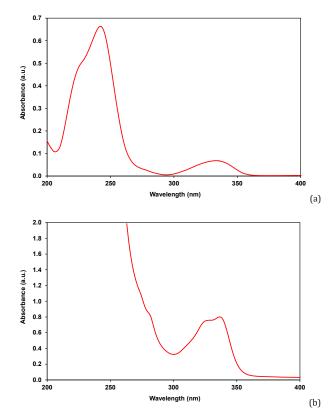


Figure 8. Experimental electronic absorption spectra of TMQ (1×10-5 M) in ethanol (a) and acetonitrile (b) at room temperature.

From Figure 8 maximum absorption wavelength bands were observed at 241, 327 nm in ethanol and 252, 336 nm in acetonitrile for the compound TMQ.

## 3.6.1. The theoretical electronic absorption spectrum of TMQ

In the UV absorption region, six absorptions at 343.11 nm (λ<sub>1</sub>), 318.73 nm (λ<sub>2</sub>), 280.85 nm (λ<sub>3</sub>) 272.70 nm (λ<sub>4</sub>), 271.24 nm ( $\lambda_5$ ), and 268.52 nm ( $\lambda_6$ ) were observed for the gas phase (Table 7). The oscillator strength (f) values corresponding to six wavelengths were 0.0026, 0.0676, 0.0156, 0.0046, 0.0252, 0.0004 oscillator strength value. In the ethanol environment, TMQ exhibited the following six wavelengths at 325.60, nm  $(\lambda_1)$ , 322.65 nm  $(\lambda_2)$ , 282.94 nm  $(\lambda_3)$ , 264.69, nm  $(\lambda_4)$ , 261.90 nm ( $\lambda_5$ ), and 257.35 nm ( $\lambda_6$ ), and the parallel oscillator strength (f) values were observed to be 0.0193, 0.0731, 0.0193, 0.0194, 0.2104, 0.1212, respectively. Acetonitrile environment of TMQ was absorbed at 326.87 nm ( $\lambda_1$ ), 324.43 nm ( $\lambda_2$ ), 284.24 nm ( $\lambda_3$ ), 265.91 nm ( $\lambda_4$ ), 262.92 nm ( $\lambda_5$ ), and 258.39 nm ( $\lambda_6$ ), and the equivalent oscillator strength (f) values were observed to be 0.0273, 0.0639, 0.0196, 0.0175, 0.2116, 0.0977.

#### 3.7. Cyclic voltammetry (CV)

In order to investigate the electrochemical properties (HOMO and LUMO) of TMQ, cyclic voltammetry (CV) measurements were carried out. Figure 9 shows cyclic voltammogram of TMQ. HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) energy levels were calculated by using the Equations (2) and (3), respectively [50-52] and given in Table 8.

$$E_{\rm g}=1240/\lambda \tag{1}$$

$$HOMO = -[4.44 + E^{OX}_{onset}] (eV)$$
<sup>(2)</sup>

$$LUMO = [HOMO + E_{Opt}] (eV)$$
(3)

where,  $E^{OX}_{onset}$  and  $E_{Opt}$  are onset oxidation potential and optical band gap respectively. The HOMO energy levels of TMQwas determined and found to be in the range -5.052 eV (v/s. Ag/AgCl).

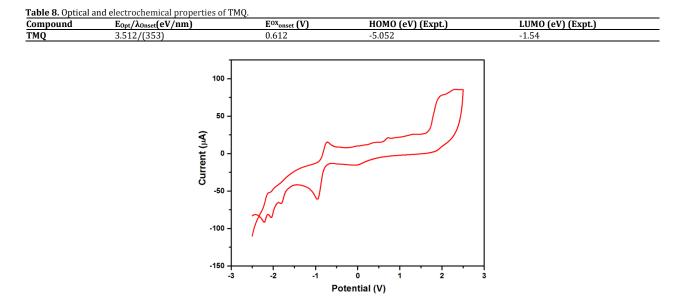


Figure 9. Cyclic voltammogram of TMQ in acetonitrile in the presence of tetrabutylammoniumhexafluorophosphate (Supporting electrolyte) at a scan rate of 100 mV/s.

From Tables 7 and 8, it was observed that the band gaps, HOMO and LUMO values obtained experimentally are approximately in close agreement with values obtained using DFT.

#### 3.8. Mulliken atomic charges and natural charges

The calculation of atomic charges plays a vital role in the application of quantum mechanical calculations to molecular systems. Mulliken charges are evaluated by determining the electron population analysis of each atom as defined in the basic functions. The charge distributions calculated by the Mulliken [53] and NBO methods for the equilibrium geometry of TMQ are given in Table 7. Atomic charges particularly that of reactive ones are very important in defining the reactive nature of molecules under study [54]. This analysis was performed at DFT/B3LYP using two methods 6-31++G (d,p) and 6-311G++(2d,p) basis set. All the hydrogen atoms have positive charges, an acceptor atom for the studied molecule. The distribution of charge on the molecule has an important influence on the vibrational spectra.Mulliken atomic charge of the carbon atoms in the neighbourhood of C22, C23 and C36 become more positive, due to surrounded by more electronegative atoms and shows that the natural atomic charges are more sensitive to the changes in the molecular structure than Mulliken's net charges [55]. C14, Cl1, N5, C17 were changed from negative to positive, due to the effect of Cl atom. Besides, C30, C31, C34 positive to negative most possibly due to electro negativity contribution from halogen (Table 9) [54].

Mulliken charges obtained by different basis sets have been compared and represented in Table 9 in order to examine the sensitivity of the calculated charges to alter in the selection of the basis set. It is interesting to note that change in the charge distribution value is observed with two different basis sets. These natural charge calculations showed the electronegative nature of the 0, N and Cl atoms. The carbon (C22) of the triazole C=0 group possess the highest positive value of 0.79993 e (6-31++G(d,p)) and 0.78821e (6-311G++ (2d,p)) resulting from its bonding to one electronegative oxygen atom. Of the N-atoms of the triazole ring, the first Natom has the least negative charge of -0.29196. In addition, all carbon atoms are negatively charged except those attached to the strong electronegative N, O and Cl atom. The oxygen atom attached to aromatic ring (O2) has the lesser negative value - 0.53951 e / -0.52973 compared with the O4 (-0.66976 e) [6-31++G (d,p)] / O4 (-0.66559 e) [6-311G++ (2d,p)] attached with the triazole ring. The electropositive nature of all the hydrogen atoms was observed. The nitrogen atom (N3) present in the quinoline ring system possesses more electronegative value -0.45714 and -0.43291.

#### 3.9. NBO analysis

Natural bond orbital (NBO) analysis provides the most precise possible 'natural Lewis structure' by utilizing details of all orbital that are mathematically chosen to consist of the highest probable percentage of the electron density (ED). NBO analysis helps us to understand the delocalization of electron density from 'Lewis occupied donor' NBOs to properly unoccupied 'non-Lewis acceptor' NBOs in the molecule. To explore the intra and inter-molecular interactions, the stabilization energies TMQ were calculated by using second-order perturbation theory. For each donor NBO (i) and acceptor NBO (j), the stabilization energy E<sup>(2)</sup> associated with electron delocalization between donor and acceptor is calculated as [56].

$$E^{(2)} = \Delta E_{ij} = q_i \frac{F(i,j)^2}{e_i - e_i}$$
(4)

Where,  $q_i \rightarrow$  donor orbital occupancy,  $E_i, E_j \rightarrow$  diagonal elements (orbital energies) and  $F(i,j) \rightarrow$  the off-diagonal NBO Fock matrix element. The complete NBO analysis and second order Fock matrix perturbation theory analysis was carried for the title molecule under study using B3LYP/6-311++G(2d,p) level of theory. In NBO analysis, the greater the  $E^{(2)}$  (stabilization energy) value, the more exhaustive is the interacttion between electron-donors and electron-acceptors i.e. the more donating tendency from electron donors to electron acceptors, and greater the extent of conjugation of the whole system. The stabilization energies  $[E^{(2)}]$  of the donor-acceptor interactions with more than 5 kcal/mol determined by second order perturbation analysis of Fock matrix of TMQ is reported in the Table 10.

Atoms	Atomic charges(Mulliken)	Natural charges	Atomic charges (Mulliken)	Natural charges
	6-31++G(d, p)	6-31++G(d, p)	6-311++G(2d, p)	6-311++G(2d, p)
Cl1	0.026991	-0.02079	-0.063774	-0.01987
02	-0.33771	-0.52973	-0.436535	-0.53951
N3	-0.0695	-0.43291	-0.200568	-0.45714
04	-0.52227	-0.66559	-0.48729	-0.66976
N5	0.30345	-0.28286	0.118766	-0.29196
N6	-0.37689	-0.29664	-0.376311	-0.3006
C7	-0.201	-0.29866	-0.253533	-0.20103
-18	0.165256	0.20343	0.141882	0.171
H9	0.160746	0.22838	0.173438	0.19262
H10	0.167261	0.20492	0.145156	0.17253
C11	-0.34359	0.31909	0.060499	0.33368
C12	-0.21804	-0.28958	-0.371064	-0.2701
H13	0.09385	0.24587	0.166663	0.21371
C14	0.154984	-0.08152	0.535227	-0.08708
C15	0.300682	-0.14415	-0.222587	-0.0684
H16	0.18063	0.2638	0.235302	0.22128
C17	1.282312	-0.11966	0.939888	-0.12958
C18	-0.71334	-0.25643	-0.714541	-0.18742
H19	0.207724	0.27264	0.209468	0.23384
H20	0.198725	0.26297	0.199435	0.22845
N21	-0.32406	-0.47188	-0.032455	-0.47685
C22	-0.03983	0.78821	0.081885	0.79993
223	-0.56993	0.14635	0.224346	0.15378
C24	0.34095	-0.25375	-0.131644	-0.2239
H25	0.198003	0.27427	0.213608	0.24405
226	-0.37709	-0.22412	-0.203351	-0.18635
127	0.118074	0.24002	0.133359	0.20402
C28	-0.23963	-0.24903	-0.366897	-0.21583
H29	0.105848	0.23851	0.121031	0.20374
C30	-0.17956	0.21024	-0.258584	0.22792
231	-0.62352	0.15616	-0.09016	0.16325
C32	-0.34019	-0.20288	-0.263201	-0.16782
H33	0.15829	0.25759	0.154558	0.22198
C34	0.208713	-0.24031	0.074353	-0.20578
H35	0.147777	0.25651	0.157561	0.221
236	0.322857	0.21428	0.125576	0.24812
137	0.176487	0.24649	0.183568	0.21291
238	0.073646	-0.2246	-0.085895	-0.18702
H39	0.121259	0.24003	0.134879	0.20421
C40	0.088516	-0.24848	-0.162534	-0.21785
H41	0.173131	0.26405	0.190477	0.23191

The orbital energy decreases due to the interaction between the doubly occupied orbitals and the unoccupied orbital, which is a suitable way to interpret the molecular structure in the electronic point of view. Several other types of parameters, such as hybridization, directionality and partial charges, can also be analysed from NBO tool.

The possible intensive interaction among the whole system in title compound, there is an intermolecular hyperconjugative interaction of N3-C30 from Cl1 of n(Cl1)  $\rightarrow \pi^*$ (N3-C30) which increases the electron density (0.36900 e) and weakens the respective bonds N3-C30 leading to stabilization of 14.45 kJ/mol. Also, there occurs predominant intermolecular hyper-conjugative interaction of C11-C12 from O2 of  $\pi(02) \rightarrow \pi^*(C11-C12)$  which increases the electron density (0.32263 e) that weakens the respective bonds C11-C12 leading to stabilization of 32.71 kJ/mol. There occurs an intermolecular hyper-conjugative interaction of C17-C30 with the electron density (0.04824 e) from N3 of  $\sigma(N3) \rightarrow \sigma^*(C17-$ C30) results in to weakening the respective bonds C17-C30 and leads to stabilization of 11.76 kJ/mol. These probable observed interactions occur as an increase in electron density in the C-C anti-bonding orbital that weakens the respective bonds. In addition another kind of hyper-conjugative interaction of N5-C22 from 04 of  $\pi(04) \rightarrow \sigma^*(N5-C22)$  which increases the electron density (0.09490e) that weakens the respective bonds N5-C22 leading to stabilization of 26.76 kJ/mol and a hyper-conjugative interaction of 04-C22 with stabilization energy of 29.65 kJ/mol occurs from N5 of  $\sigma(N5)$  $\rightarrow \sigma^*(04\text{-}C22)$  which increases the electron density (0.34442) e) that weakens the respective bonds O4-C22. Moreover, there is also intermolecular hyper-conjugative interaction of N5-C22

from N6 of  $\sigma(N6) \rightarrow \sigma^*(N5-C22)$  which increases the electron density (0.09490 e) that weakens the respective bonds N5-C22 leading to stabilization of 3.5 kJ/mol. Also, there occurs an intermolecular hyper-conjugative interaction of 04-C22 from  $\sigma(N21) \rightarrow \sigma^*(04-C22)$  which increases the electron density (0.34442 e) that weakens the respective bonds 04-C22 leading to stabilization of 26.6 kJ/mol. The successful approach of second-order perturbation theory to predict the hyper-conjugative interaction energy is adopted. Electron density delocalization between the occupied Lewis type (bond or lone pair) NBO orbital and formally unoccupied (anti bond or Rydberg) non-Lewis NBO orbital corresponds to a stabilizing donor-acceptor interaction.

The NBO analysis also describes the bonding in terms of the natural hybrid orbital which occupy a higher energy orbital n3Cl1 (-0.33084 a.u.) with considerable p-character (100.0%) and low occupation number (1.92327) and the other n1(Cl1) occupy a lower energy orbital (-0.93632 a.u.) with pcharacter (16.83%) and high occupation number (1.99365). The NBO analysis also describes the bonding in terms of the natural hybrid orbital n2(02), which occupy a higher energy orbital (-0.33302 a.u.) with considerable *p*-character (100.0%) and high occupation number (1.83506). The NBO analysis also describes the bonding in terms of the natural hybrid orbital n2(04), which occupy a higher energy orbital (-0.26529 a.u.) with considerable *p*-character (100.0%) and high occupation number (1.83581). n1N5 which occupy a higher energy orbital (-0.28207 a.u.) with considerable p-character (100.0%) and high occupation number (1.60231). n1N21 which occupy a higher energy orbital (-0.28672 a.u.)

 Table 10. Second order perturbation theory analysis of Fock matrix in NBO basis corresponding to the intra-molecular bonds of TMQusing B3LYP/6-311++G

 (2d,p) basis set.

Donor (i)	Type of bond orbital	ED/e Occupancy	Acceptor (j)	Type of bond orbital	ED/e Occupancy	Energy E(2) kcal/mol	E(i)-E(j)a.u. Energy difference	F(i,j)a.u. Polarized energy
N3-C30	σ	1.98627	N3-C31	σ*	0.02423	1.85	1.40	0.046
N3-C30	π	1.81489	C17-C30	σ*	0.04824	2.93	0.96	0.049
04-C22	σ	1.98927	N5-C22	σ*	0.09490	0.99	0.96	0.028
04-C22	π	1.98837	N5-N6	σ*	0.02298	0.93	1.21	0.030
N5-N6	σ	1.97933	N5-C23	σ*	0.03683	0.93	1.22	0.030
N5-C22	σ	1.98479	04-C22	σ*	0.34442	0.68	0.97	0.025
N6-C36	σ	1.98244	N5-C23	σ*	0.03683	3.77	1.28	0.062
C11-C12		1.97760	02-C7	σ*	0.00935	1.77	0.86	0.035
C11-C12		1.73203	C14-C15	σ*	0.02000	0.58	0.51	0.016
C11-C34		1.97116	02-C7	σ*	0.00935	4.14	0.81	0.052
C14-C15	σ	1.96937	C11-C12	σ*	0.02684	1.74	1.29	0.042
C15-C17		1.71676	N3-C30	π*	0.36900	25.19	0.26	0.074
C17-C18		1.97460	N3-C30	σ*	0.02398	2.98	1.24	0.054
C17-C30		1.97742	N3-C30	σ*	0.02398	3.06	1.31	0.057
N21-C36		1.98581	04-C22	σ*	0.34442	1.38	0.98	0.036
C23-C24		1.97099	N5-N6	σ*	0.02298	6.18	1.02	0.071
C23-C24		1.97250	N5-N6	σ*	0.02298	1.42	1.02	0.034
C31-C32		1.97425	N3-C30	σ*	0.02398	2.65	1.02	0.052
C32-C34		1.75559	C11-C12	π* σ*	0.32263	18.81	0.28	0.067
C38-C40		1.97611	N5-C23	σ* π*	0.03683	4.14	1.08	0.060
	π	1.67977	C26-C28	π* *	0.33949	18.74	0.29	0.066
P Cl1	σ	1.99365	N3-C30	σ* σ*	0.02398	0.62	1.51	0.027
LP 02	σ	1.96453	C11-C12	$\sigma^*_*$	0.02684	6.99	1.15	0.080
LP N3	σ	1.89208	C17-C30	σ*	0.04824	11.76	0.83	0.090
LP 04	σ	1.97846	N5-C22	σ*	0.09490	2.37	1.10	0.046
LP N5	σ	1.60231	04-C22	σ*	0.34442	29.65	0.42	0.101
	σ	1.94352	N5-N6	σ*	0.02298 0.34442	0.94 26.60	0.71 0.42	0.023 0.096
LP N21 <b>Fable 11</b> .				σ*	ıls.	20.00		
<b>Donor(i)</b> σN3-C30	. NBO results sho	owing the format <b>ED/e</b> 1.98627	ion of Lewis and <b>EDA%</b> 59.54	l non-Lewis orbita EDB% 40.46	ıls. NBO 0.7716(sp <sup>1.57</sup> )N	+	<b>S%</b> 38.84	<b>P%</b> 60.84
LP N21 <b>Γable 11.</b> <b>Donor(i)</b> σN3-C30 πN3-C30	. NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489	ion of Lewis and <b>EDA%</b> 59.54 56.34	l non-Lewis orbita EDB% 40.46 43.66	lls. <b>NBO</b> 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N	+	<b>S%</b> 38.84 0.00	<b>P%</b> 60.84 100.0
LP N21 <b>Fable 11.</b> <b>Donor(i)</b> 5N3-C30 πN3-C30 504-C22	. NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927	ion of Lewis and <b>EDA%</b> 59.54 56.34 70.36	l non-Lewis orbita EDB% 40.46 43.66 29.64	lls. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C	+  + )+	<b>S%</b> 38.84 0.00 10.12	<b>P%</b> 60.84 100.0 89.49
LP N21 <b>Fable 11.</b> <b>Donor(i)</b> 5N3-C30 τN3-C30 504-C22 τ04-C22	. NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927 1.98837	ion of Lewis and EDA% 59.54 56.34 70.36 65.61	l non-Lewis orbitz EDB% 40.46 43.66 29.64 34.39	lls. <b>NBO</b> 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C	+  + )+	<b>\$%</b> 38.84 0.00 10.12 29.02	<b>P%</b> 60.84 100.0 89.49 70.50
<u>Fable 11.</u> <u>Donor(i)</u> 5N3-C30 τN3-C30 τ04-C22 τ04-C22 τ04-C22 5N5-N6	. NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18	I non-Lewis orbita EDB% 40.46 43.66 29.64 34.39 44.82	lls. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.66</sup> )N	+  + )+  +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30	<b>P%</b> 60.84 100.0 89.49 70.50 72.59
LP N21 Table 11. Donor(i) 5N3-C30 τN3-C30 τO4-C22 τO4-C22 5N5-N6 5N5-C22	NBO results sho	bwing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20	I non-Lewis orbitz EDB% 40.46 43.66 29.64 34.39 44.82 36.80	NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.65</sup> )N 0.7950 (sp <sup>1.94</sup> )N	+  +  +  +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92	<b>P%</b> 60.84 100.0 89.49 70.50 72.59 65.96
LP N21 <b>Table 11. Donor(i)</b> 5N3-C30           τN3-C30           τ04-C22           τ04-C22           τN5-N6           5N5-C22           5N6-C36	. NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86	l non-Lewis orbita EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14	Ils. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.66</sup> )N 0.7950 (sp <sup>1.94</sup> )N 0.7672 (sp <sup>1.61</sup> )N	+  + )+  +  +	<b>S%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08	<b>P%</b> 60.84 100.0 89.49 70.50 72.59 65.96 61.44
<u><b>Cable 11.</b></u> <b>Cable 11.</b> <b>Donor(i)</b> 5N3-C30 τN3-C30 τO4-C22 τO4-C22 τO4-C22 5N5-N6 5N5-C22 5N5-C22 5N6-C36 5τC11-C12	. NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16	l non-Lewis orbita EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84	Ils. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.66</sup> )N 0.7950 (sp <sup>1.94</sup> )N 0.7672 (sp <sup>1.61</sup> )N 0.7082 (sp <sup>1.54</sup> )C	+  + +  +  +  +	<b>5%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35	<b>P%</b> 60.84 100.0 89.49 70.50 72.59 65.96 61.44 60.59
P N21           Cable 11.           Donor(i)           5N3-C30           tN3-C30           t004-C22           t04-C22           t04-C22           t05-N6           5N5-N6           5N6-C36           5C11-C12           t C11-C12	. NBO results sho 2	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93	l non-Lewis orbita EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84 54.07	Ils. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.66</sup> )N 0.7950 (sp <sup>1.94</sup> )N 0.7672 (sp <sup>1.54</sup> )C 0.7082 (sp <sup>1.54</sup> )C 0.6777 (sp <sup>1.00</sup> )C	+  + )+  +  +  +  +	<b>5%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00	<b>P%</b> 60.84 100.0 89.49 70.50 72.59 65.96 61.44 60.59 100.0
P N21           Table 11.           Donor(i)           xN3-C30           x04-C22           x04-C22           x05-C62           x05-C62           x06-C36           x06-C36           x01-C12           x01-C12           x01-C12	. NBO results sho 2 2	by wing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.66</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.54</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7122 (sp <sup>1.80</sup> )C	+  +  +  +  +  +  +  +  +  +	<b>5%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29
P N21           Cable 11.           Donor(i)           IN3-C30           t04-C22           t04-C22           t04-C22           t05-N6           t05-C25           t06-C36           t01-C12           t11-C12           t11-C12           t11-C12           t11-C14	NBO results sho	by wing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.9733 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.34</sup> )N           0.7672 (sp <sup>1.54</sup> )C           0.7672 (sp <sup>1.54</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7122 (sp <sup>1.80</sup> )C           0.7176 (sp <sup>2.00</sup> )C	+  +  +  +  +  +  + + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63
LP N21 <b>Fable 11. Donor(i) π</b> N3-C30 <b>π</b> N3-C30 <b>π</b> O4-C22 <b>π</b> N5-N6 <b>π</b> N5-C22 <b>π</b> N6-C36 <b>π</b> C11-C12 <b>π</b> C11-C134 <b>π</b> C11-C15 <b>π</b> C11-C17 <b>π</b> C11-C17 <b>π</b> C11-C17 <b>π</b> C11-C17	NBO results sho 2 2 4 5 7	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.97137 1.96937 1.71676	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60	I non-Lewis orbita EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84 54.07 49.28 48.51 54.40	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7082 (sp <sup>1.54</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7122 (sp <sup>1.80</sup> )C           0.7176 (sp <sup>2.00</sup> )C           0.6752 (sp <sup>1.00</sup> )C	+  +  +  +  +  +  +  +  + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0
P N21           Cable 11.           Donor(i)           JN3-C30           tN3-C30           tN3-C30           tod-C22           tod-C22           tod-C36           to1-C12           to1-C12 <t< td=""><td>NBO results sho</td><td>owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460</td><td>ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77</td><td>I non-Lewis orbitz EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84 54.07 49.28 48.51 54.40 49.23</td><td>IIS. NBO 0.7716(sp<sup>1.57</sup>)N 0.7506 (sp<sup>1.00</sup>)N 0.8388 (sp<sup>8.84</sup>)C 0.8100 (sp<sup>2.43</sup>)C 0.7428 (sp<sup>2.64</sup>)N 0.7950 (sp<sup>1.94</sup>)N 0.7672 (sp<sup>1.61</sup>)N 0.7082 (sp<sup>1.54</sup>)C 0.6777 (sp<sup>1.00</sup>)C 0.7122 (sp<sup>1.80</sup>)C 0.7126 (sp<sup>2.00</sup>)C 0.7125 (sp<sup>2.15</sup>)C</td><td>+  +  +  +  +  +  +  +  + + + + + +</td><td>S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72</td><td>P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22</td></t<>	NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77	I non-Lewis orbitz EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84 54.07 49.28 48.51 54.40 49.23	IIS. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.84</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.64</sup> )N 0.7950 (sp <sup>1.94</sup> )N 0.7672 (sp <sup>1.61</sup> )N 0.7082 (sp <sup>1.54</sup> )C 0.6777 (sp <sup>1.00</sup> )C 0.7122 (sp <sup>1.80</sup> )C 0.7126 (sp <sup>2.00</sup> )C 0.7125 (sp <sup>2.15</sup> )C	+  +  +  +  +  +  +  +  + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22
<u>P N21</u> <b>Fable 11.</b> <b>Donor(i)</b> N3-C30 τ04-C22 τ04-C	NBO results sho	bwing the format <b>ED/e</b> 1.98627 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.01)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C	+  +  +  +  +  + + + + + + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00 31.72 32.89	<b>P%</b> 60.84 100.0 89.49 70.50 72.59 65.96 61.44 60.59 100.0 64.29 66.63 100.0 68.22 67.03
P N21           Gable 11.           Donor(j)           JN3-C30           TN3-C30           TN3-C30           JO-C22           TO-C22	NBO results sho	by wing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.9837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.98581	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 63.53	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7126 (sp2.00)C           0.7125 (sp2.10)C           0.7125 (sp2.10)C           0.7126 (sp2.00)C           0.7125 (sp2.01)C           0.7970 (sp1.96)N	+  +  +  +  +  +  +  +  +  +	<b>5%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00 31.72 32.89 33.74	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14
P N21 Table 11. Donor(i) m3-C30 tN3-C30 to4-C22 to4-C15 to4	NBO results sho	by wing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.98581 1.97099	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 63.53 51.62	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           36.47           48.38	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.54</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7122 (sp <sup>1.61</sup> )N           0.7122 (sp <sup>1.61</sup> )C           0.7176 (sp <sup>2.00</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7125 (sp <sup>2.04</sup> )C           0.7970 (sp <sup>1.96</sup> )N           0.7184 (sp <sup>1.68</sup> )C	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62
P N21           Cable 11.           Donor(j)           xN3-C30           x04-C22           x05-N6           x05-N6           x05-C26           x06-C36           x011-C34           x014-C15           x014-C15           x014-C15           x014-C15           x014-C36           x014-C32           x014-C32           x014-C32           x014-C35           x012-C36           x023-C24           x023-C24           x023-C40	NBO results sho 2 2 4 5 5 6 4	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.98581 1.97099 1.97250	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 63.53 51.62 51.52	I non-Lewis orbit:           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           36.47           48.38           48.48	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.60</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7176 (sp <sup>2.00</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7125 (sp <sup>2.04</sup> )C           0.7970 (sp <sup>1.96</sup> )N           0.7184 (sp <sup>1.69</sup> )C           0.7178 (sp <sup>1.71</sup> )C	+ + + + + + + + + + + + + + + + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00 31.72 32.89 33.74 37.33 36.94	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00
<u>P N21</u> <b>Fable 11.</b> <b>Donor(i)</b> N3-C30 τN3-C30 τ04-C22 τ04-C	NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.98581 1.97099 1.97250 1.97425	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 63.53 51.62 51.52 51.17	I non-Lewis orbitz EDB% 40.46 43.66 29.64 34.39 44.82 36.80 41.14 49.84 54.07 49.28 48.51 54.40 49.23 49.23 36.47 48.38 48.48 48.83	IIS. NBO 0.7716(sp <sup>1.57</sup> )N 0.7506 (sp <sup>1.00</sup> )N 0.8388 (sp <sup>8.49</sup> )C 0.8100 (sp <sup>2.43</sup> )C 0.7428 (sp <sup>2.64</sup> )N 0.7950 (sp <sup>1.94</sup> )N 0.7672 (sp <sup>1.61</sup> )N 0.7082 (sp <sup>1.54</sup> )C 0.6777 (sp <sup>1.00</sup> )C 0.7172 (sp <sup>1.80</sup> )C 0.7172 (sp <sup>1.80</sup> )C 0.7125 (sp <sup>2.04</sup> )C 0.7125 (sp <sup>2.04</sup> )C 0.7125 (sp <sup>2.04</sup> )C 0.7125 (sp <sup>2.04</sup> )C 0.7128 (sp <sup>1.96</sup> )N 0.7178 (sp <sup>1.71</sup> )C 0.7154 (sp <sup>1.87</sup> )C	+  +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06
P N21 Cable 11. Donor(i) N3-C30 tN3-C30 t04-C22 t04-C23 t04-C3 t04-	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.98927 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96761 1.97460 1.97742 1.97551 1.97250 1.97250 1.97255 1.75559	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 63.53 51.62 51.52 51.17 49.06	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           36.47           48.38           48.48           50.94	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7128 (sp1.68)C           0.7128 (sp1.77)C           0.7124 (sp1.87)C           0.7125 (sp2.04)C	+  +  +  +  +  + + + + + + + + + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00 31.72 32.89 33.74 37.33 36.94 34.88 0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00
P N21 Table 11. Donor(i) N3-C30 tN3-C30 tN3-C30 to4-C22 to4	NBO results sho	by wing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.97581 1.97099 1.97250 1.97425 1.75559 1.97611	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.60)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7672 (sp1.61)N           0.7672 (sp1.61)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.01)C           0.7125 (sp2.01)C           0.7125 (sp2.01)C           0.7184 (sp1.68)C           0.7154 (sp1.81)C           0.7004 (sp1.91)C           0.7036 (sp1.81)C	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29
P N21           Gable 11.           Donor(i)           JN3-C30           TN3-C30           TN3-C30           JO4-C22           TO4-C22           TO4-C22           TO4-C22           TO4-C22           TO5-N6           TO1-C12           TC11-C12           TC11-C14           TC11-C15           TC11-C16           TC17-C18           TC23-C24           TC32-C34           TC32-C34           TC32-C34           TC38-C40           TC38-C40	NBO results sho	by wing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.97759 1.97250 1.97259 1.97259 1.97559 1.97611 1.67977	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 63.53 51.62 51.52 51.17 49.06	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           36.47           48.38           48.48           50.94	NBO           0.7716 (sp1-57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2-43)C           0.7428 (sp2.65)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7672 (sp1.61)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp2.04)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7184 (sp1.68)C           0.7184 (sp1.87)C           0.7154 (sp1.87)C           0.7036 (sp1.810)C           0.7036 (sp1.810)C           0.7036 (sp1.810)C           0.7036 (sp1.810)C           0.7036 (sp1.810)C           0.7036 (sp1.810)C           0.7018 (sp1.00)C	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.00
P N21 Table 11. Donor(1) rN3-C30 rN3-C30 r04-C22 r04-C23 r01-C18 r023-C24 r04-C32 r03-C32 r	NBO results sho 2 2 4 5 7 8 9 9 5 6 4 9 9 9	owing the format ED/e 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.98581 1.97099 1.97250 1.97425 1.97559 1.97611 1.67977 1.99365	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.00</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.60</sup> )C           0.6777 (sp <sup>1.00</sup> )C           0.7176 (sp <sup>2.01</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7126 (sp <sup>1.90</sup> )N           0.7184 (sp <sup>1.69</sup> )C           0.7184 (sp <sup>1.69</sup> )C           0.7184 (sp <sup>1.69</sup> )C           0.7184 (sp <sup>1.69</sup> )C           0.7004 (sp <sup>1.00</sup> )C           0.7036 (sp <sup>1.81</sup> )C           0.7018 (sp <sup>1.00</sup> )C	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           83.16	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.0           64.29           100.0           64.29           100.0           64.31           66.32           66.33           100.0           66.34           66.35           100.00           65.36           100.00           64.29           100.0           16.83
<u>P N21</u> <b>Fable 11.</b> <b>Donor(i)</b> N3-C30 τN3-C30 τ04-C22 τ04-C3 τ04-C4 τ04-C3 τ04-C4 τ04-C3 τ04-C4	NBO results sho	owing the format ED/e 1.98627 1.81489 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96761 1.97742 1.97742 1.97559 1.97425 1.97559 1.97611 1.67977 1.99365 1.9696	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7052 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7125 (sp2.15)C           0.7128 (sp1.57)C           0.7178 (sp1.71)C           0.7178 (sp1.71)C           0.7004 (sp1.80)C           0.7036 (sp1.81)C           0.7018 (sp1.00)C           sp2.00           0.7018 (sp1.00)C           sp2.00	+  +  +  +  +  +  + + + + + + + + + + +	<b>\$%</b> 38.84 0.00 10.12 29.02 27.30 33.92 38.08 39.35 0.00 35.64 33.30 0.00 31.72 32.89 33.74 37.33 36.94 34.88 0.00 35.59 0.00 83.16 0.52	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.3           99.47
P N21 Table 11. Donor(i) N3-C30 tN3-C30 tN3-C30 to4-C22 to4-C32 to4	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.98827 1.98927 1.98927 1.98244 1.97760 1.73203 1.97116 1.96760 1.71676 1.97460 1.97742 1.97559 1.97455 1.97559 1.97611 1.67977 1.99365 1.9666 1.92327	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.00)C           0.7125 (sp2.01)C           0.7125 (sp2.01)C           0.7178 (sp1.71)C           0.7178 (sp1.71)C           0.7174 (sp1.87)C           0.7018 (sp1.80)C           0.7018 (sp1.00)C           sp1.00           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           83.16           0.52           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.00           64.29           100.00
P N21 Fable 11. Donor(i) N3-C30 TN3-C30 TN3-C30 TN3-C30 TO4-C22 TO4-C32 TO4-C32 TO4-C32 TO4-C32 TO3-C32 TO3-C38 TO4	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97740 1.97742 1.97581 1.97099 1.97250 1.97425 1.75559 1.97611 1.67977 1.99655 1.96496 1.92327 1.96453	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.65)N           0.7950 (sp1.94)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.61)N           0.7125 (sp2.15)C           0.7125 (sp2.16)C           0.7125 (sp2.16)C           0.7178 (sp1.71)C           0.7178 (sp1.71)C           0.7154 (sp1.87)C           0.7036 (sp1.00)C           0.7018 (sp1.00)C           0.7018 (sp1.00)C           0.7018 (sp1.00)C           sp1.00           sp1.00           sp1.00           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           35.59           0.00           33.16           0.52           0.00           37.66	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.96           100.00           64.29           100.00           64.29           100.00           64.29           100.00           64.29           100.00           64.29           100.00           62.20
P N21 Table 11. Donor(i) N3-C30 tN3-C30 t04-C22 t04-C22 t04-C22 t04-C22 t04-C22 t04-C22 t04-C22 t04-C12 t04-C12 t04-C12 t04-C12 t04-C12 t04-C12 t04-C12 t04-C23 t04-C23 t04-C23 t02 t03 t02 t03 t02 t04 t02 t04-C34 t02 t03 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t04 t02 t02 t02 t02 t02 t02 t02 t02	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98927 1.98337 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.97750 1.97742 1.97250 1.97259 1.97259 1.97259 1.97425 1.97611 1.67977 1.99365 1.96966 1.92327 1.96453 1.83506	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.65)N           0.7950 (sp1.94)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.61)N           0.7125 (sp2.15)C           0.7125 (sp2.15)C           0.7125 (sp2.14)C           0.77176 (sp1.00)C           0.7125 (sp2.14)C           0.7126 (sp1.71)C           0.7178 (sp1.71)C           0.7154 (sp1.87)C           0.7036 (sp1.81)C           0.7018 (sp1.00)C           sp1.00           sp1.00           sp1.00           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           35.59           0.00           37.66           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           64.29           100.0           62.20           100.0
P N21 Fable 11. Donor(i) rN3-C30 rN3-C30 r04-C22 r03-C23 r02 r032-C24 r032-C34 r023-C40 r021 r022 r032-C40 r020	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97742 1.97425 1.97559 1.97425 1.97559 1.97425 1.97559 1.97425 1.97559 1.97611 1.67977 1.99365 1.99365 1.96696 1.9227 1.96453 1.83506 1.89208	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp <sup>1.57</sup> )N           0.7506 (sp <sup>1.67</sup> )N           0.7506 (sp <sup>1.67</sup> )N           0.8388 (sp <sup>8.84</sup> )C           0.8100 (sp <sup>2.43</sup> )C           0.7428 (sp <sup>2.65</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7950 (sp <sup>1.94</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.61</sup> )N           0.7672 (sp <sup>1.61</sup> )C           0.7125 (sp <sup>2.15</sup> )C           0.7125 (sp <sup>2.16</sup> )C           0.7125 (sp <sup>2.16</sup> )C           0.7125 (sp <sup>2.16</sup> )C           0.7125 (sp <sup>1.61</sup> )C           0.7126 (sp <sup>1.61</sup> )C           0.7127 (sp <sup>1.60</sup> )C           0.7128 (sp <sup>1.61</sup> )C           0.7126 (sp <sup>1.61</sup> )C           0.7127 (sp <sup>1.61</sup> )C           0.7128 (sp <sup>1.61</sup> )C           0.7184 (sp <sup>1.63</sup> )C           0.7018 (sp <sup>1.65</sup> )C           sp <sup>1.00</sup> sp <sup>1.00</sup> sp <sup>1.00</sup> sp <sup>1.00</sup> sp <sup>1.00</sup>	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           83.16           0.52           0.00           37.66           0.00           26.40	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.0           64.29           100.0           64.29           100.0           64.29           100.0           62.20           100.00           62.20           100.0           73.25
P N21 Fable 11. Donor(i) rN3-C30 rN3-C30 r04-C22 r04-C3 r04-C3 r023-C44 r038-C40 r04-C15 r023-C44 r038-C40 r04-C15 r022 r02	. NBO results sho 2 2 2 4 5 7 7 8 9 9 9 9 9	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96761 1.97742 1.97559 1.97460 1.97742 1.97559 1.97611 1.67977 1.99365 1.9696 1.92327 1.96453 1.83506 1.89208 1.97846	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7082 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7125 (sp2.04)C           0.7126 (sp1.86)C           0.7125 (sp1.96)N           0.7125 (sp2.04)C           0.7126 (sp1.96)N           0.7125 (sp2.04)C           0.7126 (sp1.97)C           0.7127 (sp1.97)C           0.7128 (sp1.96)N           0.7154 (sp1.87)C           0.7004 (sp1.90)C           0.7018 (sp1.90)C           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp2.77           sp0.64	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           33.16           0.52           0.00           37.66           0.00           36.40           60.80	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.00           64.29           100.00           64.29           100.00           62.20           100.00           62.20           100.00           62.20           100.01
P N21 Fable 11. Donor(i) N3-C30 tN3-C30 tN3-C30 tN3-C30 tN3-C30 tro4-C22 tro4	. NBO results sho 2 2 4 5 7 8 9 9 9	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97740 1.97740 1.97559 1.97651 1.67977 1.99651 1.96965 1.92327 1.96453 1.83506 1.89208 1.97846 1.97846 1.97846 1.97846 1.93881	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.00)C           0.7125 (sp2.01)C           0.7125 (sp2.10)C           0.7126 (sp1.96)N           0.7184 (sp1.68)C           0.7018 (sp1.71)C           0.7018 (sp1.81)C           0.7018 (sp1.00)C           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           37.66           0.00           37.66           0.00           26.40           60.80           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.00           64.29           100.00           62.20           100.00           62.20           100.00           62.20           100.00           62.20           100.00
LP N21 Fable 11. Donor(i) σN3-C30 πN3-C30 σO4-C22 σN5-N6 σN5-C22 σN6-C22 σN6-C36 σC4-C22 πC15-C17 σC11-C12 πC11-C12 πC11-C134 πC12-C14 πC12-C18 σC17-C18 σC23-C24 σC3-C24 σC	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98937 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97740 1.97740 1.97742 1.97559 1.97611 1.67977 1.99653 1.96453 1.83506 1.89208 1.97846 1.83581 1.60231	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.60)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7950 (sp1.94)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.91)C           0.7125 (sp2.91)C           0.7125 (sp2.10)C           0.7126 (sp1.91)C           0.7178 (sp1.71)C           0.7184 (sp1.87)C           0.7018 (sp1.01)C           0.7018 (sp1.00)C           sp1.00           sp1.00           sp1.65           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           37.66           0.00           37.66           0.00           26.40           60.80           0.00           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.0           65.26           99.47           100.00           62.20           100.0           73.25           39.11           100.00           100.00
LP N21           Fable 11.           Donor(i)           JN3-C30           πN3-C30           πN3-C30           σ04-C22           σ01-C12           σ017-C30           σ023-C40           σ023-C42           σ023-C42           σ023-C44           σ038-C40           101C1           12C11           102           1202           10104           10204	NBO results sho	owing the format <b>ED/e</b> 1.98627 1.81489 1.98927 1.98837 1.97933 1.98479 1.98244 1.97760 1.73203 1.97116 1.96937 1.71676 1.97460 1.97740 1.97740 1.97559 1.97651 1.67977 1.99651 1.96965 1.92327 1.96453 1.83506 1.89208 1.97846 1.97846 1.97846 1.97846 1.93881	ion of Lewis and EDA% 59.54 56.34 70.36 65.61 55.18 63.20 58.86 50.16 45.93 50.72 51.49 45.60 50.77 50.77 50.77 50.77 50.77 50.77 50.77 51.52 51.17 49.06 49.51	I non-Lewis orbitz           EDB%           40.46           43.66           29.64           34.39           44.82           36.80           41.14           49.84           54.07           49.28           48.51           54.40           49.23           49.23           36.47           48.38           48.48           48.83           50.94           50.49	NBO           0.7716 (sp1.57)N           0.7506 (sp1.00)N           0.8388 (sp8.84)C           0.8100 (sp2.43)C           0.7428 (sp2.66)N           0.7950 (sp1.94)N           0.7672 (sp1.61)N           0.7082 (sp1.54)C           0.6777 (sp1.00)C           0.7122 (sp1.80)C           0.7125 (sp2.00)C           0.7125 (sp2.01)C           0.7125 (sp2.10)C           0.7126 (sp1.96)N           0.7184 (sp1.68)C           0.7018 (sp1.71)C           0.7018 (sp1.81)C           0.7018 (sp1.00)C           sp1.00	+  +  +  +  +  +  + + + + + + + + + + +	S%           38.84           0.00           10.12           29.02           27.30           33.92           38.08           39.35           0.00           35.64           33.30           0.00           31.72           32.89           33.74           37.33           36.94           34.88           0.00           35.59           0.00           37.66           0.00           37.66           0.00           26.40           60.80           0.00	P%           60.84           100.0           89.49           70.50           72.59           65.96           61.44           60.59           100.0           64.29           66.63           100.0           68.22           67.03           66.14           62.62           63.00           65.06           100.00           64.29           100.00           64.29           100.00           62.20           100.00           62.20           100.00           62.20           100.00           62.20           100.00

with considerable p-character (100.0%) and high occupation number (1.61253). Thus, a very close to pure p-type lone pair orbital participates in the electron donation to the n(Cl1)  $\rightarrow$  $\pi^*(N3-C30)$ ,  $\pi(02) \rightarrow \pi^*(C11-C12)$ ,  $\sigma(N3) \rightarrow \sigma^*(C17-C30)$ ,  $\pi(04) \rightarrow \sigma^*(N5-C22)$ ,  $\sigma(N5) \rightarrow \sigma^*(04-C22)$ ,  $\sigma(N6) \rightarrow \sigma^*(N5-C22)$ ,  $\sigma(N21) \rightarrow \sigma^*(04-C22)$  interactions in the compound. The results are displayed in Table 11.

#### 4. Conclusions

In the present study, the single crystal X-Ray and DFT analysis of TMQ is reported. It is interesting to note that the optimized geometrical (DFT) results are found in good conformity with the obtained single X-ray diffraction results (XRD). MEP predicts the most reactive component in the molecule. The Hirshfeld surfaces and fingerprint plots predictted that TMQ molecule is stabilized by various intermolecular contacts such as H····H, C···C, C···H/ H···C, N···H/H···N, O···H/H···O, Cl···H/H···Cl, C···Cl/Cl···C, C···N/N···C, C···O/O···C, and Cl···O/O···Cl interactions. A complete molecular picture, stability of the molecule arising from hyper-conjugative interaction, charge delocalization and bond length have been investigated by using Natural Bond Orbital (NBO) analysis. Both experimental and theoretical HOMO and LUMO energies

determine the charge transfer within the molecule and the difference between HOMO and LUMO energy has supported the chemical and bioactivity properties of TMQ. Mulliken atomic charge of the carbon atoms in the neighborhood of C22, C23 and C36 become more positive indicating the direction of delocalization and also showed that the natural atomic charges are more sensitive to the changes in the molecular structure than Mulliken's net charges.

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#### Supporting information S

CCDC-1828103 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/, or by emailing data request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

#### Disclosure statement 📭

Conflict of interests: The authors declare that they have no conflict of interest.

Author contributions: All authors contributed equally to this work.

Ethical approval: All ethical guidelines have been adhered.

Sample availability: Sample of the compound is available from the author.

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#### References

[1]. Rastelli, E. J.; Truong, N. T.; Coltart, D. M. Org. Lett. 2016, 18, 5588-5591.

- Kim, S. H.; Kaplan, J. A.; Sun, Y.; Shieh, A.; Sun, H. L.; Croce, C. M.; [2]. Parquette, J. R. Chem. Eur. J. 2015, 21, 101-105.
- [3]. Forkuo, A. D.; Ansah, C.; Boadu, K. M.; Boampong, J. N.; Ameyaw, E. O.; Gyan, B. A.; Ofori, M. F. Malar. J. 2016, 15, 1-12.
- [4]. Gaurav, A.; Singh, R. Med. Chem. Res. 2014, 23, 5008-5030.
- [5]. Lee, H. W.; Lee, H. S.; Park, J. H.; Cheong, J. J.; Kwon, H. B.; Kim, K. O.; Song, H. H. J. Appl. Biol. Chem. 2015, 58, 1-3 [6].
- Wise, R.; Andrews, J. M.; Edwards, L. J. Antimicrob. Agents. Chemother. 1983, 23, 559-564 [7]. Brown, C. E.; Mc Nulty, J.; Bordon, C.; Yolken, R.; Jones-Brando, L. Org.
- Biomol. Chem. 2016, 14, 5951-5955. [8].
- Musiol, R.; Serda, M.; Hensel-Bielowka, S.; Polanski, J. Curr. Med. Chem. 2010, 17, 1960-1973. [9]. Luo, Z. G.; Zeng, C. C.; Wang, F.; He, H. Q.; Wang, C. X.; Du, H. G.; Hu, L.
- M. Chem. Res. Chin. Univ. 2009, 25, 841-845. [10].
- Liu, H.; Dong, Y.; Zhang, B.; Liu, F.; Tan, C.; Tan, Y.; Jiang, Y. Sensors Sens. Actuator B-Chem. 2016, 234, 616-624.
- Prodi, L.; Bargossi, C.; Montalti, M.; Zaccheroni, N.; Su, N.; Bradshaw, J. [11]. S.; Izatt, R. M.; Savage, P. B. J. Am. Chem. Soc. 2000, 122, 6769-6770.
- [12]. El Ashry, E. S. H.; Awad, L. F.; Soliman, S. M.; Moaty, M. N. A. A.; Ghabbour, H. A.; Barakat, A. J. Mol. Struct. 2017, 1146, 432-440.
- [13]. Almasirad, A.; Tabatabai, S. A.; Faizi, M.; Kebriaeezadeh, A.; Mehrabi, N.; Dalvandi, A.; Shafiee, A. Bioorg. Med. Chem. Lett. 2004, 14, 6057-6059
- [14]. El Akri, K.; Bougrin, K.; Balzarini, J.; Faraj, A.; Benhida, R. Bioorg. Med. Chem. Lett. 2007. 17. 6656-6659
- Karthikeyan, M. S.; Holla, B. S.; Kumari, N. S. Eur. J. Med. Chem. 2008, [15]. 43. 309-314.
- Somagond, S. M.; Kamble R. R.; Kattimani, P. P.; Shaikh, S. J.; Dixit, S. [16]. R.; Joshi, S. D.; Devarajegowda, H. C. Chemistry Select 2018, 3, 2004-2016.
- [17]. Yang, F.; Zhang, X. L.; Sun, K.; Xiong, M. J.; Xia, P. F.; Cao, Z. J. Synth. Met. 2008, 158, 988-992.
- Maiti, A.; Svizhenko, A.; Anantram, M. P. Phys. Rev. Lett. 2002, 88, [18]. 1268051-1268054
- [19]. Zhou, D.; Ma, D.; Wang, Y.; Xianchun Liu; Xinhe Bao; Chem. Phys. Lett. 2003, 373, 46-51.
- [20]. Leconte, J.; Markovits, A.; Skalli, M. K.; Minot, C.; Belmajdoub, A. Surf. Sci. 2002. 497. 194-204. Wang, J.; Liu, C.; Fang, Z.; Liu, Y.; Han, Z.; J. Phys. Chem. B 2004, 108, [21].
- 1653-1659. Koch, W.; Holthausen, M. C. A.; Chemists Guide to Density Functional [22].
- Theory, Wiley-VCH, Weinheim, New York, Chichester, 2000. Parr, R. G.; Yang, W. T.; Density-Functional Theory of Atoms and [23].
- Molecules, Oxford University Press, New York, 1989. [24].
- Szafran, M.; Komasa, A.; Adamska, E. B. J. Mol. Struct. Theochem. 2007, 827, 101-107.
- [25]. Rigaku, Crystal Clear SM Expert 2. 0 r15. Software for data collection and processing. Rigaku Corporation, Tokyo, Japan. 2011.
- [26]. Sheldrick, G. M. Acta. Cryst. A 2008, 64, 112-122.
- [27]. Spek, A. L. Acta. Cryst. A 1990, 46, C34.
- Macrae, C. F.; Bruno, I. J.; Chisholm, J. A.; Edging-ton, P. R.; McCabe, P.; [28]. Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; van deStreek, J.; Wood, P. A. J. Appl. Crystallog. 2008, 41, 466-470.
- [29] McKinnon, J. J.; Spackman, M. A.; Mitchell, A. S.; J. Acta. Crystallogr. B 2004, 60, 627-668.
- [30]. Spackman, M. A.; Jayatilaka, D. Cryst. Engg. Comm. 2009, 11, 19-32.
- [31].
- Spackman, M. A.; McKinnon, J. J. Cryst. Eng. Comm. 2002, 4, 378-392. Madan, K. S.; Manjunath, B. C.; Lingaraju, G. S.; Abdoh, M. M. M.; [32]. Sadashiva, M. P.; Lokanath, N. K. Crystal. Struct. Theor. Appl. 2013, 3, 124-131.
- [33]. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Gaussian 09, Revision B. 01, Wallingford CT, 2010.
- [34]. Hartley, D.; Kidd, H. (Eds.), The Agrochemicals Handbook, Royal Society of Chemistry, Unwin Brothers Ltd., Old Woking Surrey, United Kingdom, 1983.
- Gerhartz, W.; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed., [35]. VCH Publishers, Deerfield Beach FL, 1985.
- Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F.; NBO [36]. Version 3. 1, Gaussian Inc., Pittsburgh, PA, 2000-2003.
- [37]. Dennington, R.; Keith T.; Millam J.; GaussView, Version 5, Semichem Inc., Shawnee Mission KS, 2009.

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- [38]. Mckinnon, J. J.; Mitchell, A. S.; Spackman, M. A. Chem. Eur. J. 1998, 4, 2136-2144.
- [39]. Spackman, M. A.; Jayatilaka, D. Cryst. Eng. Comm. 2009, 11, 249-253.
- [40]. Hirshfeld, F. L. Theor. Chim. Acta. 1977, 44, 129-138.
- [41]. Spackman, M. A.; Byrom P. G. Chem. Phys. Lett. 1997, 267, 215-220.
- [42]. Rohl, A. L.; Moret, M.; Kaminsky, W.; Claborn, K.; McKinnon, J. J.; Kahr, B. Cryst. Growth Des. 2008, 8, 4517-4525.
- [43]. Wolff S. K.; Grimwood D. J.; McKinnon J. J.; Turner M. J.; Jayatilaka D.; Spackman M. A. Crystal Explorer, the University of Western Australia, Australia, 2012.
- [44]. Skovsen, I.; Christensen, M.; Clausen, H. F.; Overgaard, J.; Stiewe, C.; De gupta, T.; Mueller, E.; Spackman, M. A.; Iversen, B. B. *Inorg. Chem.* 2010, 49, 9343-9349.
- [45]. Xavier, R. J.; Dinesh, P. Spectrochim. Acta A 2014, 118, 999-1011.
- [46]. Scrocco, E.; Tomasi, J. Adv. Quant. Chem. **1978**, *103*, 115-193.
- [47]. Luque, F. J.; Lopez, J. M.; Orozco, M. Theor. Chem. Acc. 2000, 103, 343-345.
- [48]. Politzer, P.; Murray, J. S.; in: D. L. Beveridge; R. Lavery (Eds.), Theoretical Biochemistry and Molecular Biophysics: A

Comprehensive Survey, Protein, Adenine Press, Schenectady, New York, 2, 1991.

- [49]. Scrocco, E.; Tomasi, J. Curr. Chem. 1973, 7, 95-170.
- [17] Berockumrak, N.; Pansay, S.; Namuangruk, S.; Kaewin, T.; Jungsuttiwong S.; Sudyoadsuk; T.; Promarak V. *Eur. J. Org. Chem.* 2013, 29, 6619-6623.
- [51]. Kotchapadist, P.; Prachumrak, N.; Sunonnam, T.; Namuangruk, S.; Sudyoadsuk, T.; Keawin, T.; Jungsuttiwong, S.; Promarak, V. Eur. J. Org. Chem. 2015, 3, 496-505.
- [52]. Deshapande, N.; Belavagi N. S.; Sunagar M. G.; Gaonkar S.; Pujar G. H.; Wari M. N.; Inamdar S. R.; Khazi I. A. M. *RSC Adv.* **2015**, *5*, 86685-86696.
- [53]. Mulliken, R. S. J. Chem. Phys. **1955**, 23, 1833-1840.
- [54]. Kose, E.; Atac, A.; Bardak, F. J. Mol. Struct. 2018, 1163, 147-160.
   [55]. Benzon, K. B.; Varghese, H. T.; Yohannan-Panicker, C.; Pradhan, K.;
- [55]. Benzon, K. B.; Varghese, H. T.; Yohannan-Panicker, C.; Pradhan, K.; Bipransh, K. T.; Ashis, K. N.; Van-Alsenoy, C. Spectrochim. Acta A 2015, 146, 307-322.
- [56]. Weinhold, F.; Eric, D. Glendening, NBO 6. 0 Program Manual, University of Wisconsin, Madison, Wisconsin 53706, 2013.



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