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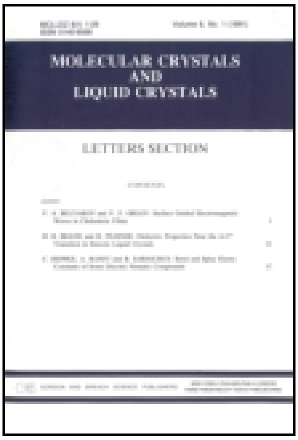

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Synthesis, Crystal Structure, and Characterization of New 2,4,5-Triphenyl Imidazole: 4,5-Diphenyl-2-(3,4,5-trimethoxyphenyl)-1H-imidazole

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Published online: 30 Dec 2013.

To cite this article: S. Viveka , M. Prabhuswamy , Dinesha , N. K. Lokanath & G. K. Nagaraja (2014) Synthesis, Crystal Structure, and Characterization of New 2,4,5-Triphenyl Imidazole: 4,5-Diphenyl-2-(3,4,5-trimethoxyphenyl)-1H-imidazole, Molecular Crystals and Liquid Crystals, 588:1, 83-94, DOI: 10.1080/15421406.2013.821933

To link to this article: http://dx.doi.org/10.1080/15421406.2013.821933

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Mol. Cryst. Liq. Cryst., Vol. 588: pp. 83–94, 2014
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ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2013.821933

Synthesis, Crystal Structure, and Characterization of New 2,4,5-Triphenyl Imidazole: 4,5-Diphenyl-2-(3,4,5-trimethoxyphenyl)-1*H*-imidazole

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The substituted triarylimidazole, $C_{24}H_{22}N_2O_3$, was prepared from the three-component one-pot condensation reaction and the product was crystallized by using dimethylformamide. The structure of the compound was confirmed by elemental analysis, FT-IR, thermogravimetric analysis (TGA), UV-Visible and single-crystal X-ray diffraction. The compound crystallizes in the monoclinic crystal system in the space group $P2_1/c$ with unit cell parameters $a = 10.509(3)$ Å, $b = 18.748(5)$ Å, $c = 22.016(6)$ Å, $\beta = 90.844(5)^\circ$, and $Z = 8$. The crystal structure of the compound was stabilized by the inter-molecular interactions of types N–H···N, C–H···O, and C–H···N, and intra-molecular interactions of the type C–H···O. The structure also involves C–H···π interactions.

Keywords Crystal structure; crystallization; FTIR spectrum; imidazole; intermolecular interactions; multicomponent reaction; thermo gram

1. Introduction

Imidazole is a planar five-member ring system with 3C and 2N atom in 1 and 3 positions. The compound is classified as aromatic due to the presence of a sextet of π-electrons, consisting of a pair of electrons from the protonated nitrogen atom and one from each of the remaining four atoms of the ring. Imidazole derivatives are very interesting class of heterocyclic compounds because they are found in many pharmacologically active substances [1]. The simple and substituted imidazoles are known for their biologically active therapeutics, glucagon receptor antagonists, and proton pump inhibitor omeprazole [2,3]. Imidazole derivatives exhibit antiviral, antifungal, and antihelmitic pesticidal and herbicidal properties [4–6]. Triarylimidazole compounds have gained the remarkable importance due to their widespread biological activities and their uses in the synthetic chemistry. In addition, they are used in photography as photosensitive compound [7].

Because of their great importance, many synthetic strategies have been developed. In 1882, Radziszewski and Japp reported the first synthesis of the imidazole from 1,2-dicarbonyl compound, various aldehydes, and ammonia to obtain the 2,4,5-triphenyl imidazoles [8,9] via multicomponent reactions (MCRs). For the preparation of 2,4,5-triphenyl imidazoles, numbers of simple, highly efficient, and versatile methods are reported in

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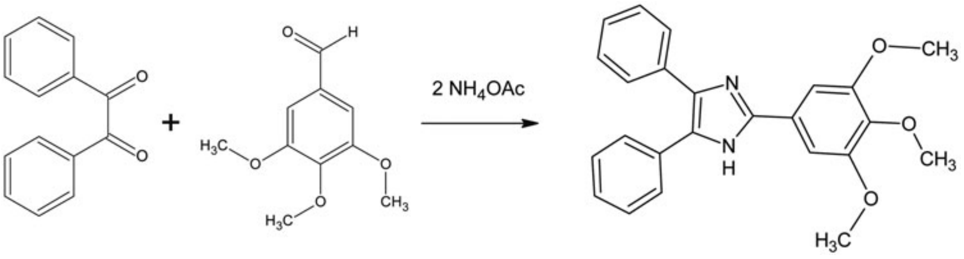

Scheme 1. Synthesis of 4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)-1H-imidazole.

the literature [10]. Prompted by the above reports we have attempted to synthesize new triarylimidazole, and characterization was done by the single-crystal X-ray diffraction, elemental Analysis, UV-Visible Spectra, FT-IR, and thermogravimetric analysis (TGA). Crystal structure of some of the similar compound is reported in the literature [11,12].

2. Experimental

2.1 Materials and Methods

All chemicals were purchased commercially and used without prior purification. Infrared spectra were recorded on a Shimadzu FT-IR spectrophotometer in the range 400–4000 cm^{-1} using the KBr pellets. A TA-SQT Q600 thermogravimetric analyzer was used to obtain TGA curve under nitrogen atmosphere with a heating rate of 20°C min^{-1}. The UV-Vis spectrum was recorded in Shimadzu UV-2550 UV-Visible spectrophotometer. Elemental analysis was carried out by using VARIO EL-III (Elementar 10 Analysensysteme GmBH).

2.2 Synthesis of Compound 4,5-Diphenyl-2-(3,4,5-trimethoxyphenyl)-1H-imidazole

Benzil (1 mmol), 3,4,5-trimethoxy benzaldehyde (10 mmol), and ammonium acetate (20 mmol) were dissolved in boiling glacial acetic acid and refluxed for 5–6 h (Scheme 1). The reaction progress was monitored by TLC. After the completion of reaction, the reaction mixture was poured into ice-water and the obtained compound was recrystallized from dimethylformamide.

The product was formed as white crystals (3.86 g, 87%) [m.p. 163°C–165°C].

3. Results and Discussion

3.1 Elemental Analysis

In order to confirm the chemical composition of the synthesized compound Carbon (C), Hydrogen (H) and Nitrogen (N) analysis was carried out. The experimental and calculated percentages of C, H, and N are given in Table 1. The differences between experimental and calculated percentages of C, H, and N were very close to each other and within the experimental errors. This confirms the formation of the product in the stoichiometric proportion.

Table 1. Elemental analysis for $C_{24}H_{22}N_2O_3$

Element	Experimental (%)	Calculated (%)
Carbon	74.57	74.59
Nitrogen	7.22	7.25
Hydrogen	5.70	5.74

3.2 *UV-Vis Spectral Analysis*

The UV-Vis spectrum of the compound is shown in Fig. 1. The UV-Vis spectrum was recorded by using dimethylformamide as a solvent. From the graph, it was observed that the compound shows an absorption peak at 313 nm. The transmittance of the compound is due to the π-π^* transition of the constituent group. There was no absorption peak between 360 nm and 900 nm in the entire visible region. Hence, the material may be useful for optoelectronic applications.

3.3 *Thermogravimetric Analysis (TGA)*

The compound decomposes mainly in two stages on heating between 30°C and 450°C as shown in Fig. 2. There was no weight loss observed up to 140°C, which shows the absence of moisture in the crystal. A weight loss of around 9% occurs between 140°C and 240°C, which is indicative of the loss of one molecule of $-OCH_3$ from a compound. The remaining part of the molecule is stable up to 310°C.

In the second stage, about 70% weight loss occurs between 310°C and 410°C. This weight loss accounts for the removal of two molecules of $-OCH_3$, three phenyl rings. Above 500°C, 17% of the residue was left out, which was due to the charring of carbon. Thus, the TGA study confirms the formation of the compound in the stoichiometric ratio.

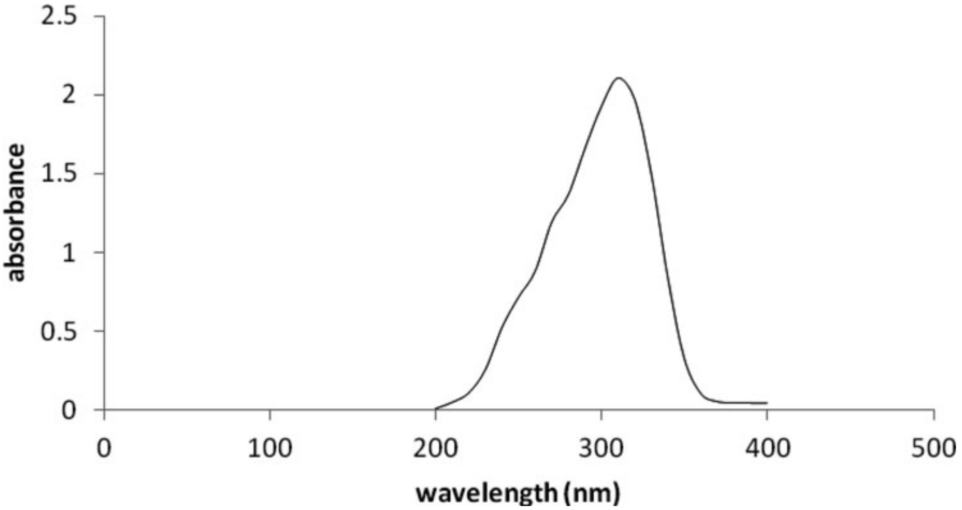

Figure 1. UV-visible spectrum of the crystal.

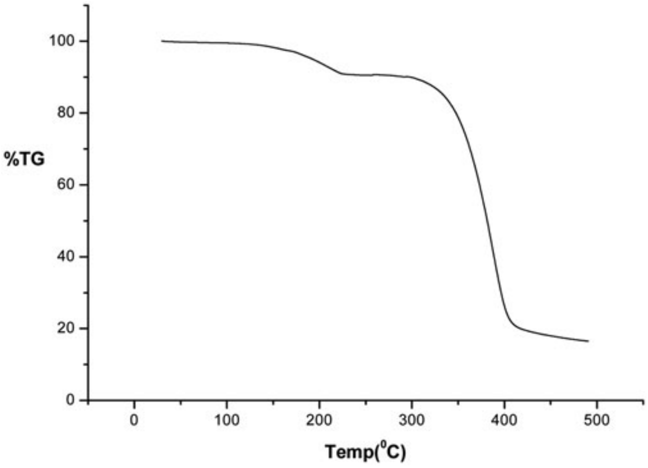

Figure 2. TGA curve of the crystal.

3.4 FT-IR Spectral Analysis

The FT-IR spectrum of the crystal structure is shown in Fig. 3. The peak at 3352 cm^{-1} was in correspondence to the N—H asymmetric stretching vibration. The peaks observed at 2920 cm^{-1} and 2833 cm^{-1} were assigned to the C—H stretching, 1126 cm^{-1} and 1002 cm^{-1}

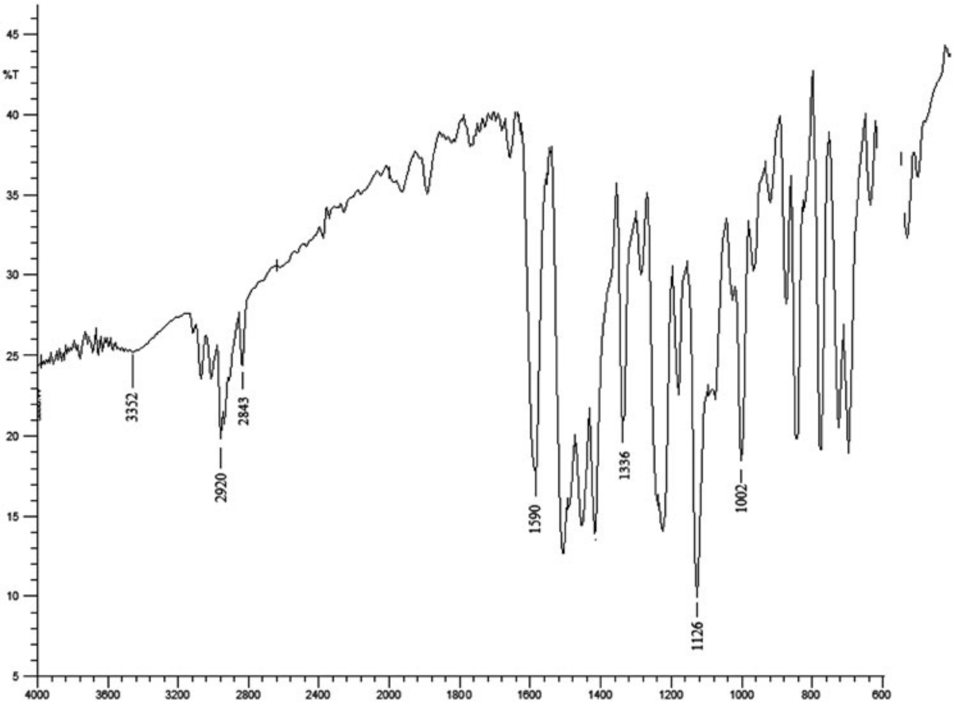

Figure 3. FTIR spectrum of the crystal.

Table 2. Crystal data and structure refinement

CCDC deposition number	931147
Empirical formula	$C_{24}H_{22}N_2O_3$
Formula weight	386.44
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	$a = 10.509(3)$ Å, $\alpha = 90^\circ$ $b = 18.748(5)$ Å, $\beta = 90.844(5)^\circ$ $c = 22.016(6)$ Å, $\gamma = 90^\circ$
Volume	4337(2) $Å^3$
Z, Calculated density	8, 1.184 Mg m^{-3}
Absorption coefficient	0.079 mm^{-1}
$F_{(000)}$	1632
Crystal size	$0.23 \times 0.20 \times 0.18$ mm
Theta range for data collection	1.85^0–25.35^0
Limiting indices	$-12 \le h \le 12, -22 \le k \le 22, -26 \le l \le 26$
Reflections collected/unique	40879/7940 [R(int) = 0.0573]
Completeness to theta = 25.35	99.9%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7940/0/529
Goodness of fit on F^2	1.088
Final R indices [$I > 2$ sigma(I)]	$R1 = 0.0706$, $wR2 = 0.1834$
R indices (all data)	$R1 = 0.0943$, $wR2 = 0.1993$
Largest diff. peak and hole	0.734 and −0.296 e$Å^{-3}$

are due to C—O stretching vibration, 1336 cm^{-1} assigned for the aromatic amines (C—N), and 1590 cm^{-1} for the C=N stretching.

3.4 Single Crystal X-Ray Diffraction Method

Single crystal of suitable size of the title compound was selected for data collection. X-ray intensity data were collected on Oxford Xcalibur Eos (Nova) CCD diffractometer with X-ray generator operating at 50 kV and 1 mA, using MoK_α radiation ($\lambda = 0.7107$ Å). Data were collected for 606 frames per set with different settings of φ (0°, 90°, 180°), keeping the sample to detector distance of 60.62 mm and the 2θ value fixed at 25°. A complete data set is reduced using the software CrysAlis PRO [13]. The structure was solved by direct methods and refined by full-matrix least squares method on F^2 using SHELXS and SHELXL programs [14]. All hydrogen atoms were positioned geometrically and refined using a riding model.

The geometrical calculations were carried out using the program PLATON [15]. The molecular and packing diagrams were generated using the software MERCURY [16]. The crystal data and structure refinement details are reported in Table 2.

The ORTEP diagram of the molecules A and B of the compound with 30% probability displacement thermal ellipsoids is shown in Figs. 4 and 5, respectively.

Table 3. Selected bond lengths (Å), angles (°), and torsion angles (°) of the title compound

Selected bond lengths (Å) and bond angles (°)		Selected torsion angles (°)	
N(1B)-C(2B)	1.331 (3)	N(1B)-C(2B)-C(18B)-C(19B)	18.2 (4)
N(1B)-C(5B)	1.383 (3)	N(3B)-C(2B)-C(18B)-C(19B)	−162.3 (3)
N(3A)-C(2A)	1.333 (3)	N(1B)-C(2B)-C(18B)-C(23B)	−160.4 (3)
N(3A)-C(4A)	1.382 (3)	N(3B)-C(2B)-C(18B)-C(23B)	19.1 (4)
N(1A)-C(2A)	1.356 (3)	C(7B)-C(6B)-C(5B)-C(4B)	48.1 (4)
N(1A)-C(5A)	1.377 (3)	C(11B)-C(6B)-C(5B)-C(4B)	−130.1 (3)
N(3B)-C(2B)	1.353 (3)	C(7B)-C(6B)-C(5B)-N(1B)	−137.4 (3)
N(3B)-C(4B)	1.371 (3)	C(11B)-C(6B)-C(5B)-N(1B)	44.4 (3)
O(1A)-C(20A)	1.368 (3)	N(3A)-C(2A)-C(18A)-C(23A)	−23.1 (4)
O(1A)-C(24A)	1.411 (4)	N(1A)-C(2A)-C(18A)-C(23A)	160.0 (3)
O(3A)-C(22A)	1.361 (3)	N(3A)-C(2A)-C(18A)-C(19A)	154.4 (3)
O(3A)-C(26A)	1.404 (4)	N(1A)-C(2A)-C(18A)-C(19A)	−22.5 (4)
O(2A)-C(21A)	1.369 (3)	C(25A)-O(2A)-C(21A)-C(20A)	−121.0 (3)
O(2A)-C(25A)	1.429 (4)	C(25A)-O(2A)-C(21A)-C(22A)	63.1 (4)
O(3B)-C(22B)	1.367 (4)	N(3B)-C(4B)-C(12B)-C(13B)	39.1 (4)
O(3B)-C(26B)	1.424 (4)	C(5B)-C(4B)-C(12B)-C(13B)	−142.2 (3)
O(1B)-C(20B)	1.362 (4)	N(3B)-C(4B)-C(12B)-C(17B)	−140.3 (3)
O(1B)-C(24B)	1.422 (6)	C(5B)-C(4B)-C(12B)-C(17B)	38.3 (4)
C(21B)-O(2B)	1.371 (4)	N(1A)-C(5A)-C(6A)-C(11A)	130.8 (3)
O(2B)-C(25B)	1.221 (10)	C(4A)-C(5A)-C(6A)-C(11A)	−46.3 (5)
C(2B)-N(1B)-C(5B)	105.8 (2)	N(1A)-C(5A)-C(6A)-C(7A)	−46.6 (4)
C(2A)-N(3A)-C(4A)	106.2 (2)	C(4A)-C(5A)-C(6A)-C(7A)	136.3 (3)
C(2A)-N(1A)-C(5A)	108.3 (2)	N(3A)-C(4A)-C(12A)-C(17A)	137.1 (3)
C(2B)-N(3B)-C(4B)	108.4 (2)	C(5A)-C(4A)-C(12A)-C(17A)	−41.5 (4)
N(1B)-C(2B)-N(3B)	110.8 (2)	N(3A)-C(4A)-C(12A)-C(13A)	−38.8 (4)
N(1B)-C(2B)-C(18B)	125.5 (2)	C(5A)-C(4A)-C(12A)-C(13A)	142.6 (3)
N(3B)-C(2B)-C(18B)	123.6 (2)	C(22B)-C(21B)-O(2B)-C(25B)	−91.2 (8)
N(3A)-C(2A)-N(1A)	110.6 (2)	C(20B)-C(21B)-O(2B)-C(25B)	91.9 (8)
N(3A)-C(2A)-C(18A)	124.1 (2)		
N(1A)-C(2A)-C(18A)	125.2 (2)		
C(20A)-O(1A)-C(24A)	117.6 (2)		
C(22A)-O(3A)-C(26A)	117.8 (2)		
N(3B)-C(4B)-C(5B)	105.4 (2)		
N(3B)-C(4B)-C(12B)	121.6 (2)		
N(1A)-C(5A)-C(4A)	105.5 (2)		
N(1A)-C(5A)-C(6A)	122.5 (2)		
N(1B)-C(5B)-C(6B)	120.5 (2)		
C(21A)-O(2A)-C(25A)	116.5 (2)		
O(2A)-C(21A)-C(20A)	118.9 (2)		
O(2A)-C(21A)-C(22A)	121.5 (2)		
O(1A)-C(20A)-C(21A)	115.1 (2)		
O(1A)-C(20A)-C(19A)	124.2 (2)		

(Continued on next page)

Table 3. Selected bond lengths (Å), angles (°), and torsion angles (°) of the title compound *(Continued)*

Selected bond lengths (Å) and bond angles (°)		Selected torsion angles (°)
N(3A)-C(4A)-C(5A)	109.4 (2)	
N(3A)-C(4A)-C(12A)	120.0 (2)	
C(22B)-O(3B)-C(26B)	118.0 (2)	
O(3A)-C(22A)-C(23A)	124.7 (2)	
O(3A)-C(22A)-C(21A)	115.2 (2)	
O(3B)-C(22B)-C(23B)	124.1 (3)	
O(3B)-C(22B)-C(21B)	115.6 (3)	
C(20B)-O(1B)-C(24B)	117.9 (3)	
O(1B)-C(20B)-C(19B)	124.0 (3)	
O(1B)-C(20B)-C(21B)	115.8 (3)	
O(2B)-C(21B)-C(22B)	120.2 (3)	
O(2B)-C(21B)-C(20B)	120.3 (3)	
C(25B)-O(2B)-C(21B)	122.3 (6)	

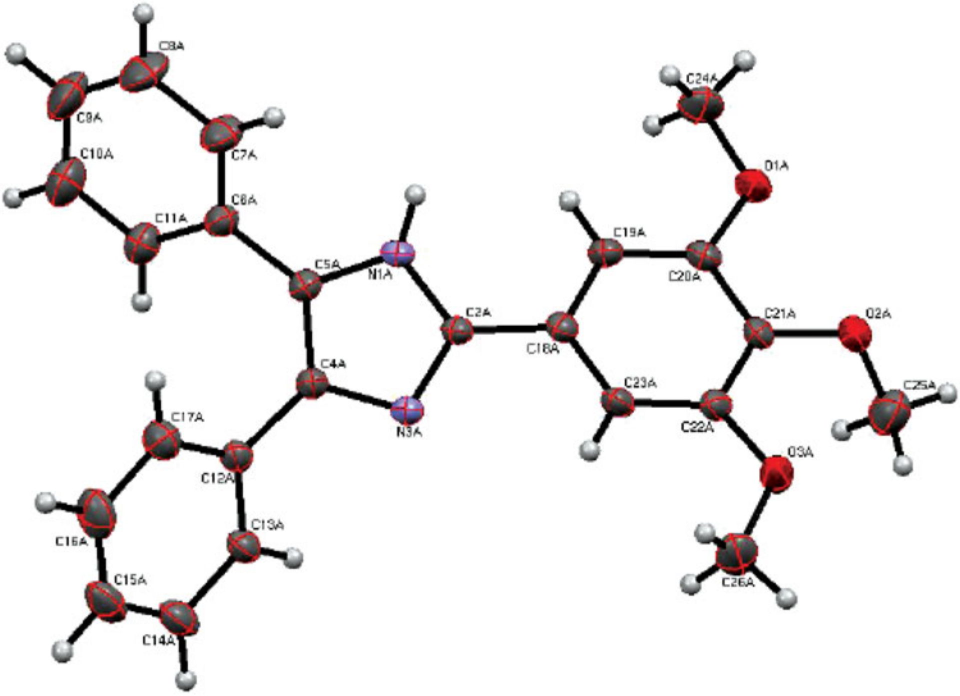

Figure 4. The ORTEP diagram of the molecule A of the title compound with 30% probability displacement thermal ellipsoids.

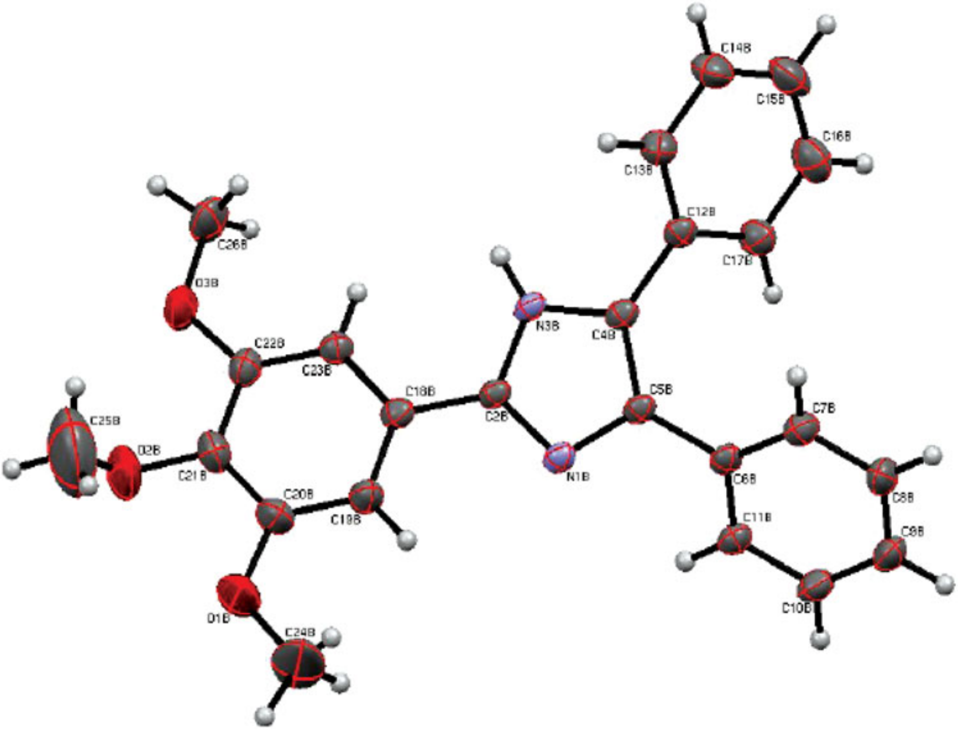

Figure 5. The ORTEP diagram of the molecule B of the title compound with 30% probability displacement thermal ellipsoids.

The packing of molecules when viewed down *a*-axis, *b*-axis, and *c*-axis are given in Figs. 6, 7, and 8, respectively, and selected bond lengths (Å), angles (°), and torsion angles (°) of the title compound are shown in Table 3.

Two molecules are present in the asymmetric unit, consisting of an imidazole ring, two phenyl rings, and a methoxy substituted phenyl ring. The imidazole ring is planar with a maximum deviation of −0.002(2) Å for the atom C(2A) in molecule **A** and −0.003(2) Å for the atom C(2B) in molecule **B**.

The methoxy substituted phenyl ring forms a dihedral angle of 23.69(14)° in molecule **A** and 18.65(14)° in molecule **B** with respect to imidazole ring, corresponding to axial position. However, phenyl ring C(6A)-C(7A)-C(8A)-C(9A)-C(10A)-C(11A) of molecule **A** and phenyl ring C(6B)-C(7B)-C(8B)-C(9B)-C(10B)-C(11B) of molecule **B** are in bisectional positions with respect to imidazole ring N(1A)-C(2A)-N(3A)-C(4A)-C(5A) of molecule **A** and imidazole ring N(1B)-C(2B)-N(3B)-C(4B)-C(5B) of molecule **B**, as confirmed by the dihedral angles 46.90(17)° and 46.22(14)° respectively, which deviates from the dihedral angle value of 68.2(3)° reported earlier for the molecular structure 1-(4-Chlorophenyl)-4,5-diphenyl-2-(3,4,5-trimethoxyphenyl)-1H-imidazole [17].

A dihedral angle of 40.21(15)° between phenyl ring C(12A)-C(13A)-C(14A)-C(15A)C(16A)-C(17A) and the imidazole ring N(1A)-C(2A)-N(3A)-C(4A)-C(5A) of molecule **A** and dihedral angle of 38.79(15)° between phenyl ring C(12B)-C(13B)-C(14B)-C(15B)C(16B)-C(17B) and imidazole ring N(1B)-C(2B)-N(3B)-C(4B)-C(5B) in molecule **B** show that they have occupied the bisectional positions in both molecules **A** and **B**.

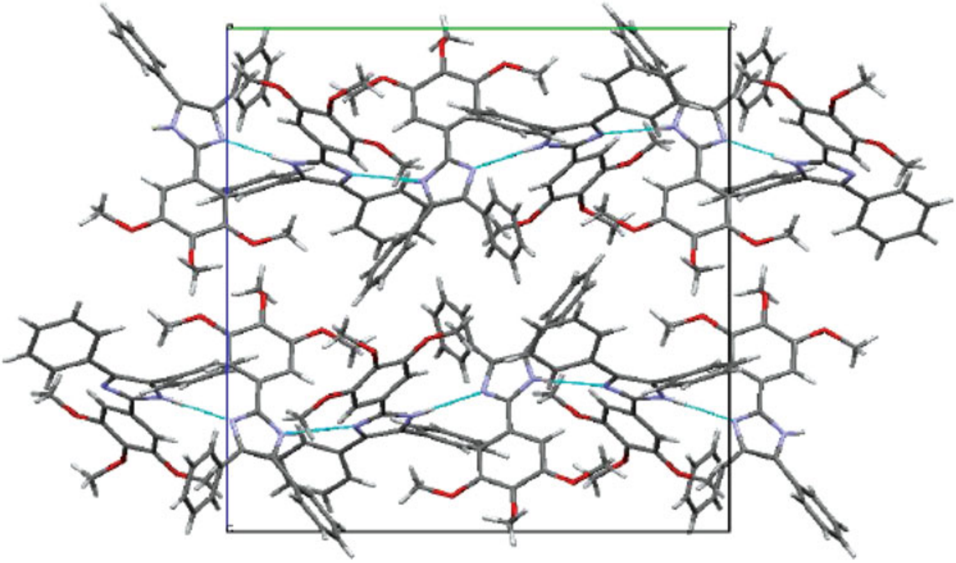

Figure 6. Packing of molecules when viewed down *a*-axis.

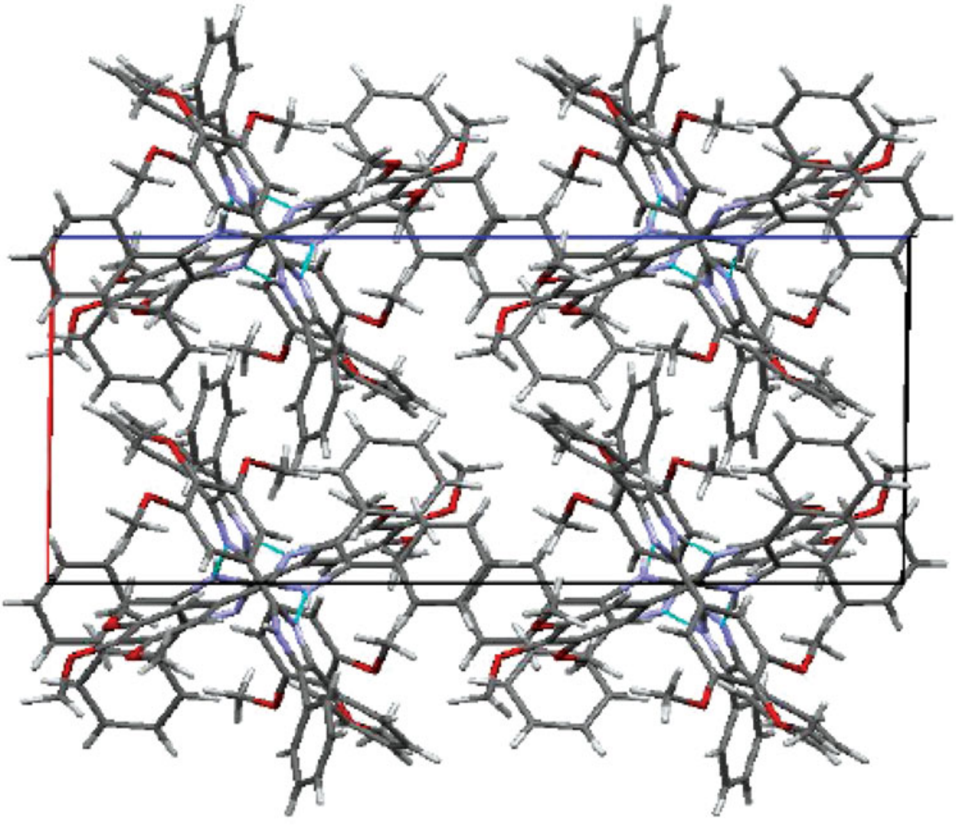

Figure 7. Packing of molecules when viewed down *b*-axis.

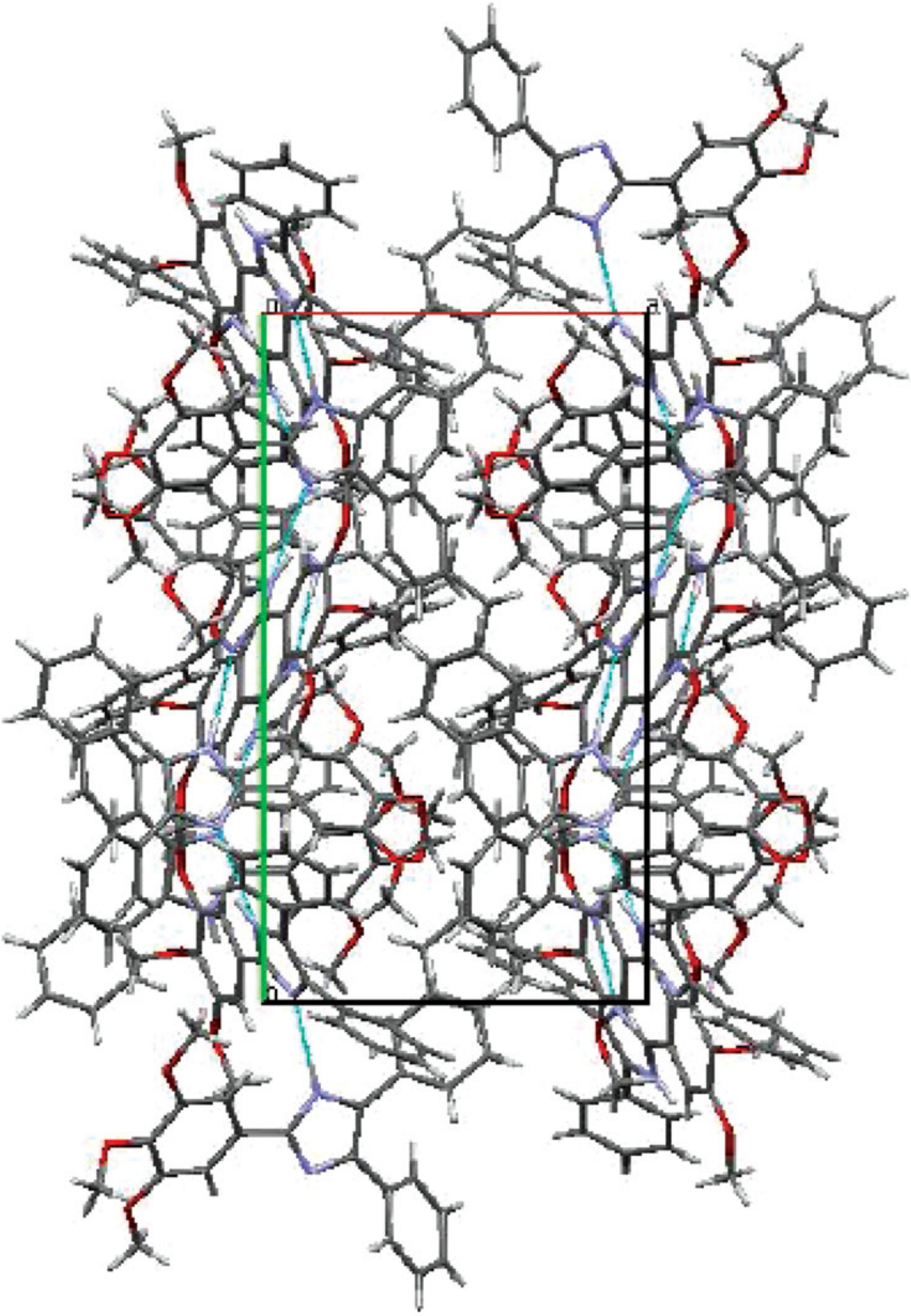

Figure 8. Packing of molecules when viewed down *c*-axis.

Table 4. Hydrogen bond geometry [Å, °]

D—H···A	d(D—H)	d(H···A)	d(D···A)	<(DHA)
N(1A)-H(1A)···N(1B)^{i}	0.86	2.07	2.930(3)	178
N(3B)-H(3B)···N(3A)	0.86	2.10	2.912(3)	158
C(10B)-H(10B)···O(2A)^{ii}	0.93	2.58	3.181(4)	123
C(23B)-H(23B)···N(3A)	0.93	2.51	3.411(3)	163
C(25A)-H(25A)···O(3A)*	0.96	2.44	2.889(5)	108

*Intra-molecular hydrogen bond interaction.

Note. Symmetry codes: *(i). −x, −1/2+y, 1/2−z; (ii). 1−x, 1/2+y, 1/2−z.*

These values of dihedral angle do not deviate much from 41.7(1)°, reported earlier for the molecular structure 2-(2-methylphenyl)-4,5-diphenyl-1H-imidazole [18]. A dihedral angle of 83.69(14)° between imidazole rings in molecule **A** and in molecule **B** shows that they are approximately orthogonal to each other.

The molecular structure shows C_g–C_g interaction between the ring C(6A)-C(7A)-C(8A)-C(9A)-C(10A)-C(11A) and C(6B)-C(7B)-C(8B)-C(9B)-C(10B)-C(11B) with a shortest centroid–centroid distance of 4.963(2) Å and symmetry code *–x, –1/2+y, 1/2−z.*

The molecule also involves C—H···π_{centroid} interactions; C(26A)-H(26C)···$\pi_{\text{(N1B-C2B-N3B-C4B-C5B)}}$, H···$\pi_{\text{centroid}}$ = 2.65 Å, C—π_{centroid} = 3.433(4) Å, C(26A)-H(26C)···π_{centroid} = 139° and C(13B)-H(13B)···$\pi_{\text{(C12A-C13A-C14A-C15A-C16A-C17A)}}$, H···$\pi_{\text{centroid}}$ = 2.93 Å, C—π_{centroid} = 3.827(4) Å, C(13B)-H(13B)···π_{centroid} = 162° with symmetry code *x, y, z*. Hydrogen bond geometry [Å,°] is given in Table 4.

An intra-molecular interaction C(25A)-H(25A)···O(3A) forms a nonplanar six membered ring C(21A)-C(22A)-O(3A)-H(25A)-C(25A)-O(2A) fused with a methoxy substituted phenyl ring in molecule **A**. In the crystal lattice of the title compound, each molecule is involved in N—H···N hydrogen bond interaction, thus giving a rippled one-dimensional chains with a base vector [0 1 0].

4. Conclusions

Single crystal was grown by slow evaporation method. The elemental analysis confirms the formation of the compound in a stoichiometric ratio. The UV-Vis spectrum reveals the properties of the crystals. TGA was carried out to study the thermal behavior of the crystal. The FTIR spectrum characterizes the presence of various functional groups. The single crystal X-ray diffraction study indicates that the compound crystallizes in monoclinic system.

Acknowledgments

The authors gratefully acknowledge the UGC and DST-PURSE for the financial assistance. They also thank Mangalore University, USIC, and MICROTONE Centre for their instrumental facilities.

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