

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/260383135>

# Thermal and Crystallographic Studies of 1-(2-Fluoro-4-Nitrophenyl)-4-(Prop-2-yn-1-yl)Piperazine Single Crystal

ARTICLE in PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES, INDIA - SECTION A · MARCH 2014

Impact Factor: 0.24 · DOI: 10.1007/s40010-013-0102-8

---

READS

33

## 4 AUTHORS, INCLUDING:



Satish K Awasthi

University of Delhi

61 PUBLICATIONS 812 CITATIONS

[SEE PROFILE](#)



Chiranjeev Sharma

University of Delhi

7 PUBLICATIONS 19 CITATIONS

[SEE PROFILE](#)



Gunjan Pandey

Indian Institute of Technology (Banaras Hin...)

4 PUBLICATIONS 13 CITATIONS

[SEE PROFILE](#)

## Thermal and Crystallographic Studies of 1-(2-Fluoro-4-Nitrophenyl)-4-(Prop-2-yn-1-yl)Piperazine Single Crystal

Satish Kumar Awasthi · Chiranjeev Sharma ·  
Monika Yadav · Gunjan Pandey

Received: 17 October 2012 / Revised: 11 October 2013 / Accepted: 17 October 2013 / Published online: 11 January 2014  
© The National Academy of Sciences, India 2014

**Abstract** 1-(2-Fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine was synthesized and single crystals were grown successfully by slow evaporation solution growth technique at room temperature. The compound was characterized by FTIR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR. From X-ray crystallography the crystal structure is monoclinic having a space group  $\text{P}2_1/\text{c}$  and the corresponding lattice parameters,  $a = 9.7366(8)$  Å,  $b = 17.9148(13)$  Å,  $c = 7.5270(6)$  Å and  $\beta = 102.397(8)$ °. Packing studies of compound reveal the presence of several intermolecular interactions viz., C–H···O hydrogen bonding, C(aryl)–H···π interactions and stacking interactions of aromatic rings which stabilize the crystal lattice. The thermal stability of single crystal was determined by TG–DTA and DSC.

**Keywords** Crystallography · Piperazine · Single crystal · Hydrogen bonding · Stacking · Thermal analysis

### Introduction

Piperazine ring is of critical importance as a scaffold in one or more of the major drug classes and is the key pharmacophoric element in design, synthesis, and biological evaluation of novel therapeutic agents. Piperazine containing molecules are known to possess various biological activities. They have been reported as antivirals for

effectively inhibiting human immunodeficiency virus (HIV-1) and human rhinovirus (HRV-3) infection [1, 2]. They show in vitro inhibitory activity on human platelet aggregation [3] and as antifilarial agents with macrofilaricidal, microfilaricidal, female-sterilizing and larvicidal efficacy [4]. They are also identified as serotonergic agents [5] and melatonergic MT2 selective agents [6]. Further, piperazine containing compounds are also known as analgesic, anti-inflammatory [7], antipsychotic [8], antidepressant [9], antifungal [10], antihypertensive [11] and hypnotic [12]. Fluoroquinolones are widely used antibacterial agent which also contain piperazine at position 7 in the quinoline scaffold [13]. Piperazine is also a starting substrate for further molecular exploration to design and synthesize new compounds with wide biological activities.

Motivated by recent results [13–16] in our laboratory we started with two-fold objectives: first is the design, synthesis and characterization of new drug molecules and second is the X-ray crystal studies of small organic molecules. Herein, we report the synthesis, spectroscopic characterization and crystallographic studies of hitherto unknown 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine. Thermal studies including differential scanning calorimeter (DSC), thermogravimetric analysis (TGA) and differential thermal analysis (DTA) have also been done.

### Materials and Methods

All solvents and reagents were obtained commercially and used as received.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR data were collected using JEOL GS-400 model FT NMR spectrometer and processed with its Delta software. The chemical shifts in spectra were measured in parts per million (ppm) on the delta ( $\delta$ ) scale relative to the resonance of the solvent

**Electronic supplementary material** The online version of this article (doi:10.1007/s40010-013-0102-8) contains supplementary material, which is available to authorized users.

S. K. Awasthi (✉) · C. Sharma · M. Yadav · G. Pandey  
Chemical Biology Laboratory, Department of Chemistry,  
University of Delhi, Delhi 110007, India  
e-mail: satishpna@gmail.com; skawasthi@chemistry.du.ac.in

peak ( $\text{CDCl}_3$  signal as reference,  $^1\text{H} = 7.19$  ppm,  $^{13}\text{C} = 77.0$  ppm). FT-IR spectra was recorded neat in the range of 600–4,000  $\text{cm}^{-1}$  at room temperature using a Perkin Elmer Spectrum 400 FT-IR spectrometer. Melting point was recorded by open capillary method on Buchi M-560 melting point apparatus.

#### Synthesis of 1-(2-Fluoro-4-Nitrophenyl)Piperazine

Synthesis of 1-(2-fluoro-4-nitrophenyl)piperazine was carried out according to the procedure reported by Khalaj et al. [17]. In a 100 ml round bottom flask, 1.2 g (7.5 mmol) of 3,4-difluoronitrobenzene was dissolved in 15 ml acetonitrile followed by addition of 1.6 g (18.5 mmol) piperazine. The mixture was refluxed for 3 h. It was cooled and left undisturbed overnight to allow the precipitation of unreacted piperazine. The precipitate was removed and the solution was concentrated in vacuo to afford an orange solid, yield = 80 %, mp 68–70 °C.

#### Synthesis of 1-(2-Fluoro-4-Nitrophenyl)-4-(Prop-2-yn-1-yl)Piperazine

Propargyl bromide (0.54 g, 4.5 mmol) was slowly added to a mixture of 1-(2-fluoro-4-nitrophenyl)piperazine (0.67 g, 3 mmol) and  $\text{K}_2\text{CO}_3$  (0.81 g, 6.3 mmol) in DMF (5 ml) at 0 °C. The mixture was heated at 60 °C and stirred for 24 h. After completion of reaction, as observed by TLC, the reaction mixture was poured into ice-cold water and the product was separated by simple filtration using Buchner funnel, yield = 77 %, mp 94–96 °C. A schematic diagram depicting the synthetic route is shown in Scheme 1.

#### Crystal Growth

X-ray quality single crystals were grown in a borosilicate glass vials of 20 ml size, 57 mm height, 28 mm diameter by the slow evaporation solution growth technique at room temperature. Briefly, 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine (ca. 15 mg) was dissolved in 5 ml

$\text{CHCl}_3$  and it was carefully filtered at room temperature using fine pore Whatman filter paper 42. The filtered solution was kept at room temperature for few days and block shaped red single crystals suitable for X-ray analysis was harvested from the mother liquor.

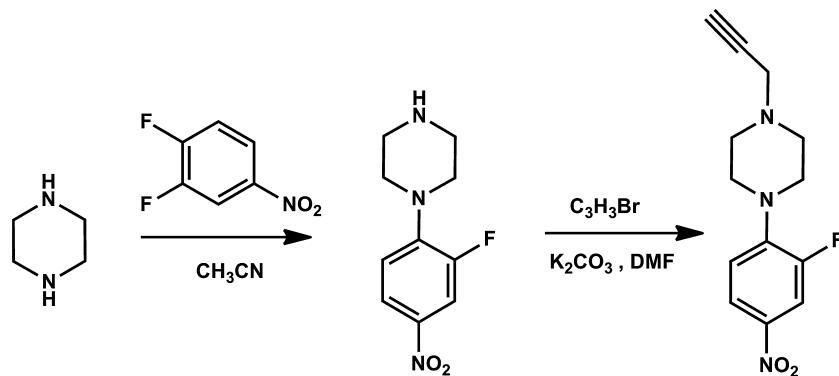
#### Results and Discussion

Spectroscopic studies reveal the formation of 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine single crystal.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and FTIR spectrum are given in supplementary material. Crystallographic studies were done on crystals grown in chloroform. The X-ray data were collected by a Bruker D8 single crystal X-ray diffractometer (Apex II). The crystals were subjected to X-ray intensity diffraction studies. Data was collected in an Oxford Diffraction Xcalibur CCD diffractometer with graphite monochromated Mo  $\text{K}\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293 (2) K. The intensity of a total number of 10,841 reflections were recorded in the range of 3.0°–26.4°, out of which 2,612 were independent reflections. The structure was solved by direct method using SHELXL-97 and refined by full matrix least-squares method on F2 (SHELXL-97) to a R value of 0.049. All calculations were carried out using the WinGX package of the crystallographic program and PLATON. Program ORTEP-3, Diamond and Mercury were used to generate molecular graphics.

#### Spectroscopic Characterization

A triplet at 2.23 ppm in  $^1\text{H}$  NMR alongwith signals at 78.18 and 73.66 ppm in  $^{13}\text{C}$  NMR confirms the presence of terminal alkyne. The signals for carbon of aromatic ring attached with fluoro, nitro and nitrogen atom of piperazine ring appear downfield in  $^{13}\text{C}$  NMR at 151.75, 140.59 and 145.41 ppm respectively. Other aromatic carbons are seen at 121.08, 117.15 and 112.47 ppm. The methylene hydrogen atoms of piperazine ring show two distinct triplets at 3.28 and 2.68 ppm. The doublet at 3.32 ppm corresponds

**Scheme 1** Synthesis of 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl) piperazine



to the two hydrogen atom of the propargyl group at C-11. The  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum of compound shows the following peaks:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$ : 7.91 (dd, 1H), 7.84 (dd, 1H), 6.85 (t, 1H,  $J = 8.70$  Hz), 3.32 (d, 2H,  $J = 2.29$ ), 3.28 (t, 4H,  $J = 4.81$ ), 2.68 (t, 4H, 4.81), 2.23 (t, 1H,  $J = 2.52$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 400 MHz)  $\delta$ : 151.75, 145.41, 140.59, 121.08, 117.15, 112.47, 78.18, 73.66, 51.46, 49.47, 46.83.

FT-IR spectra also support the findings of  $^1\text{H}$  and  $^{13}\text{C}$  NMR. The characteristic absorption bands are consistent with the functional groups present in the molecule. The  $sp$  hybridized C–H stretching of terminal alkyne appears at  $3,295\text{ cm}^{-1}$  and C≡C stretching occurs at  $2,344\text{ cm}^{-1}$ . A weak peak at  $3,087\text{ cm}^{-1}$  is due to the  $sp^2$  C–H stretching of aromatic ring, ring stretch absorptions occur in pair at  $1,604$  and  $1,453\text{ cm}^{-1}$ . Peaks at  $600$ – $900\text{ cm}^{-1}$  correspond to the 1,2,4-substituted benzene ring. The nitro group shows two strong bands at  $1,514$  and  $1,384\text{ cm}^{-1}$  due to asymmetric and symmetric stretching vibrations. The  $sp^3$  C–H of methylene groups of the piperazine ring show assymetric and symmetric stretching vibrations at  $2,920$  and  $2,840\text{ cm}^{-1}$  respectively.

### X-ray Diffraction Studies

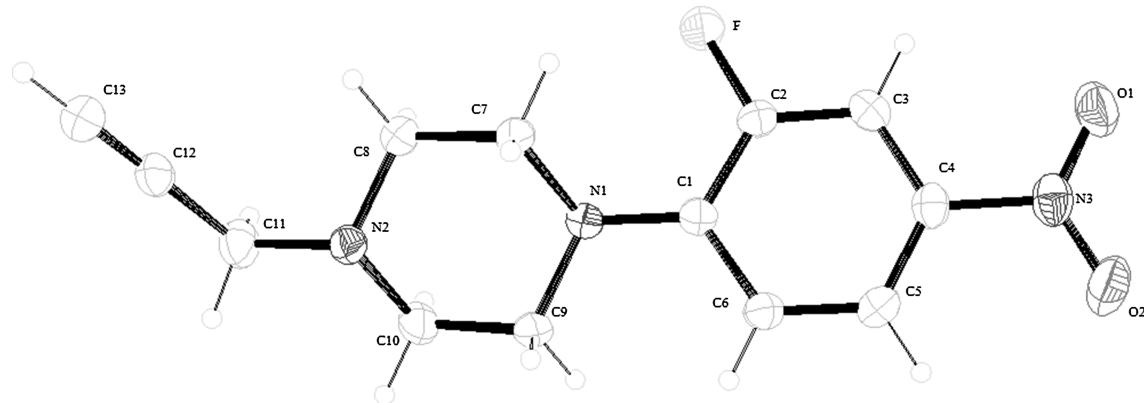
The crystal structure of the titled compound is shown in Fig. 1. The compound crystallized is monoclinic with  $P2_1/c$  space group having lattice parameters,  $a = 9.7366(8)\text{ \AA}$ ,  $b = 17.9148(13)\text{ \AA}$ ,  $c = 7.5270(6)\text{ \AA}$  and  $\beta = 102.397(8)^\circ$ . The crystallographic data and structure refinement details are given in Table 1.

A planar benzene ring is present in the molecule consisting of a fluoro and nitro groups. Another plane passes through N3–C4–C1(benzene ring)–N1–N2(piperazine ring)–C11(alkyne side chain) inclined at  $64.77^\circ$  from the benzene ring. The piperazine ring adopts a chair conformation and bridges the alkyne side chain with aromatic

**Table 1** Crystal data and structure refinement

Crystal data	Molecular formula $\text{C}_{13}\text{ H}_{14}\text{ F N}_3\text{ O}_2$
CCDC No. 880634	Space group $P2_1/c$
$M_r = 263.27$	Mo K $\alpha$ radiation, $\lambda = 0.71073\text{ \AA}$
$D_x = 1.364\text{ g cm}^{-3}$	$V = 1282.32(17)\text{ \AA}^3$
$a = 9.7366(8)\text{ \AA}$	$\mu = 0.104\text{ mm}^{-1}$
$b = 17.9148(13)\text{ \AA}$	$T = 293(2)\text{ K}$
$c = 7.5270(6)\text{ \AA}$	$F(000) = 552.0$
$\beta = 100.369(7)^\circ$	
$Z = 4$	
Data collection	
Oxford diffraction Xcalibur Sapphire3 diffractometer	Reflections with $I > 2\sigma(I) = 2200$
$\theta_{\max} = 26.4^\circ$ , $\theta_{\min} = 3.0^\circ$	$R_{\text{int}} = 0.021$
$h = -12$ – $12$	Absorption correction: multi-scan
$k = -22$ – $22$	$T_{\min} = 0.959$ , $T_{\max} = 0.969$
$l = -9$ – $9$	Measured reflections = 10,841
	Independent reflections = 2,612
Refinement	
$R[F^2 > 2\sigma(F^2)] = 0.049$	$(\Delta/\sigma)_{\max} = 0.05$
$wR(F^2) = 0.191$	
$S = 0.67$	$\Delta\rho_{\max/min} = 0.17\text{ e \AA}^{-3}$
Unique reflections = 2,612	$\Delta\rho_{\min} = -0.24\text{ e \AA}^{-3}$
Parameters = 172	Restraints = 0

ring. Further, the alkyne side chain lies in a different plane. Although the  $sp$  hybridized C13 carbon atom shows  $180^\circ$  angle between C12–C13–H13. However, C12 shows a slight deviation from the expected linear geometry as C11–C12–C13 is  $178.7(2)^\circ$ , which is perhaps due to the C–H $\cdots$  $\pi$  interaction of C13. The nitro group shows typical



**Fig. 1** Ortep diagram of 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine drawn at 30 % thermal probability

**Table 2** Selected geometric parameters: lengths and angles (Å, °)

F–C2	1.353 (2)	N2–C11	1.468 (2)
N2–C8	1.450 (2)	O1–N3	1.226 (2)
N2–C10	1.457 (2)	N3–O2	1.220 (2)
C10–N2–C11	109.54 (14)	N3–C4	1.449 (2)
O2–N3–O1	122.56 (18)	O2–N3–C4	119.20 (18)
C12–C11	1.461 (3)	O1–N3–C4	118.23 (18)
C12–C13	1.170 (3)	C12–C13–H13	180
C8–N2–C10	108.86 (15)	C13–C12–C11	178.7 (2)
C8–N2–C11	111.00 (15)	O1–N3–C4–C5	179.38 (18)
C9–N1–C1–C6	−2.6 (2)	O2–N3–C4–C3	179.14 (18)
C7–N1–C1–C6	133.53 (18)	O1–N3–C4–C3	−1.5 (3)
C9–N1–C1–C2	174.14 (17)	C8–N2–C10–C9	59.7 (2)
C7–N1–C1–C2	−49.8 (2)	C11–N2–C10–C9	−178.73 (17)
C1–N1–C7–C8	166.00 (16)	N1–C9–C10–N2	−57.4 (2)
C9–N1–C7–C8	−55.2 (2)	N1–C7–C8–N2	58.4 (2)
C10–N2–C8–C7	−59.7 (2)	C11–N2–C8–C7	179.63 (16)

bond lengths viz., N3–C4 [1.449 (2) Å], N3–O1 [1.226 (2) Å] and N3–O2 [1.220 (2) Å] of aromatic nitro compounds [18]. A list of selected geometric parameters: lengths and angles are given in Table 2.

The study of crystal structure of the titled compound reveals several intermolecular interactions viz., C–H···O hydrogen bonding, C(aryl)–H···π interactions and stacking interactions of aromatic ring. Two oxygen atoms of nitro group participate in hydrogen bonding (Fig. 2). The hydrogen bond involving oxygen atom of nitro group and hydrogen atom of terminal alkyne H13···O1 ( $d = 2.442$  Å) is slightly shorter than the hydrogen bond with the aryne hydrogen atom H7B···O2 ( $d = 2.708$  Å). Terminal alkyne also has the propensity for hydrogen bond like interactions and show C–H···π interactions between π system of alkyne –C≡C– bond and the hydrogen atoms of aromatic rings (Fig. 3) [19, 20]. A bifurcated C–H···π bond is observed

between C13 atom of one molecule and the H3 and H6 atoms of other two molecules with almost similar bond distances C13–H6 ( $d = 2.831$  Å) and C13–H3 ( $d = 2.841$  Å).

The packing diagram along c-axis shows helical symmetry as shown in Fig. 4. The helical sheets appear to be arranged in parallel fashion. Each helical sheet comprises of a pair of molecules with very special arrangement of aromatic rings overlapping partially with the stacking distance 3.533 Å, which is similar to the van der Waals distance for the carbon skeleton [21]. The distance between the centroids of two stacked benzene rings projected on a plane and defined by atoms of one ring is 2.38 Å. The inclination or tilt of one ring plane to other is 0°. Therefore, it presents an example of antiparallel stacking. Consequently, the alkyne groups appear to cluster together. It looks like a zipper which closes at C13–H13 and opens at C11 keeping the two molecules together, which are further connected to another molecules by stacking interactions. The zipper and antiparallel stacking interaction alternates resulting in an infinite helical sheets along the crystallographic c-axis.

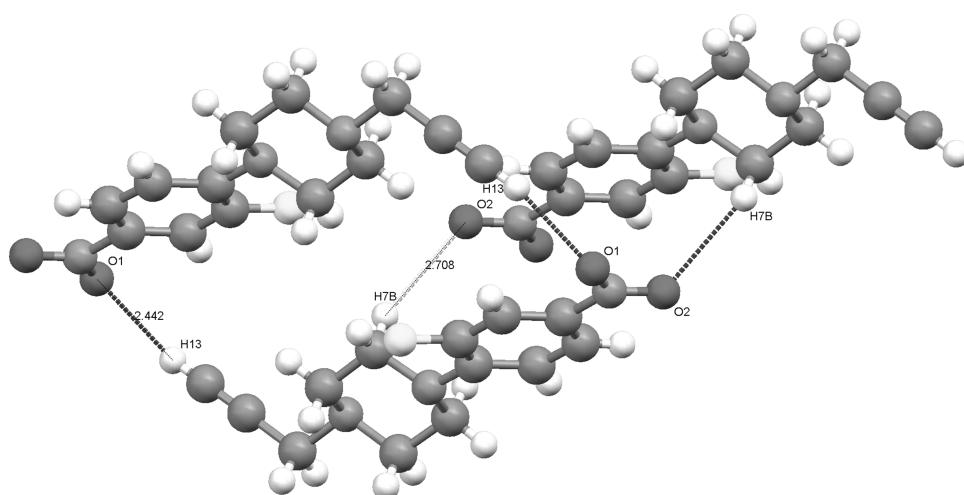
The crystal structure of the titled compound also confirms the absence of intramolecular interactions and lattice held solvent or water molecule in the unit cell of the determined structure.

## Thermal Studies

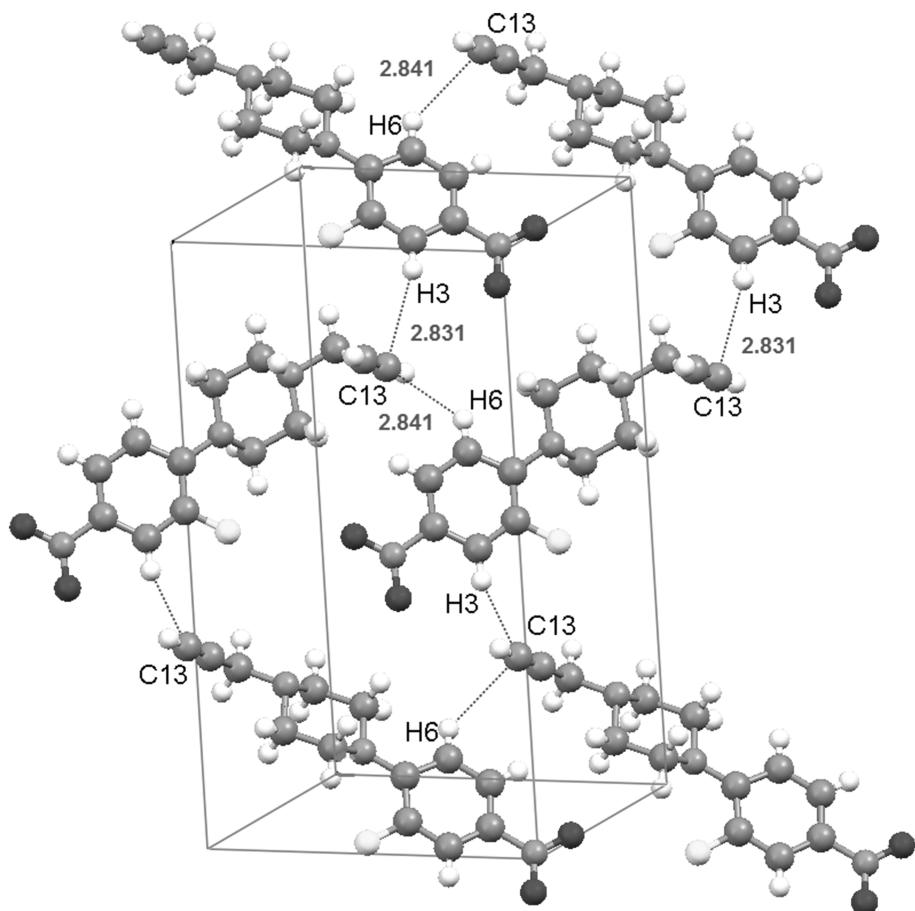
### Thermogravimetric Analysis

TG–DTA data was collected on Perkin Elmer Instrument, Diamond TG/DTA in an open ceramic pan after equilibration at 25 °C followed by a 10 °C min<sup>−1</sup> ramp up to 900 °C. The TGA and DTA measurements were performed in flowing dry nitrogen at 20 ml min<sup>−1</sup> on 6.235 mg sample. The result of TG–DTA measurements is shown in Fig. 5. DTA curve shows an endothermic peak at 97.58 °C

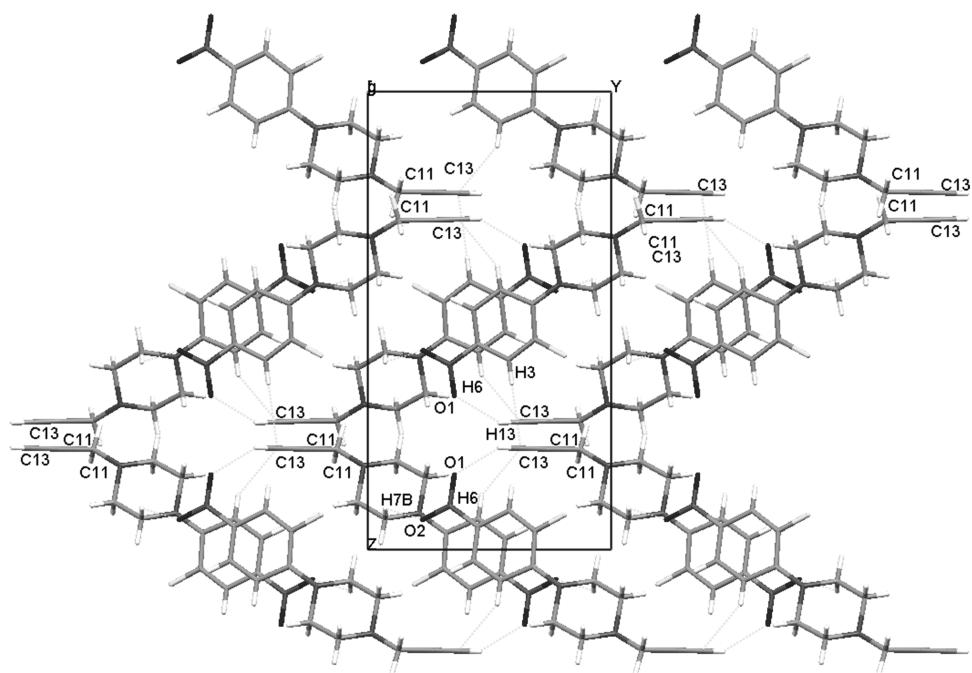
**Fig. 2** C–H···O hydrogen bonding in 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine



**Fig. 3** C–H···ii interactions in the 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl) piperazine crystals

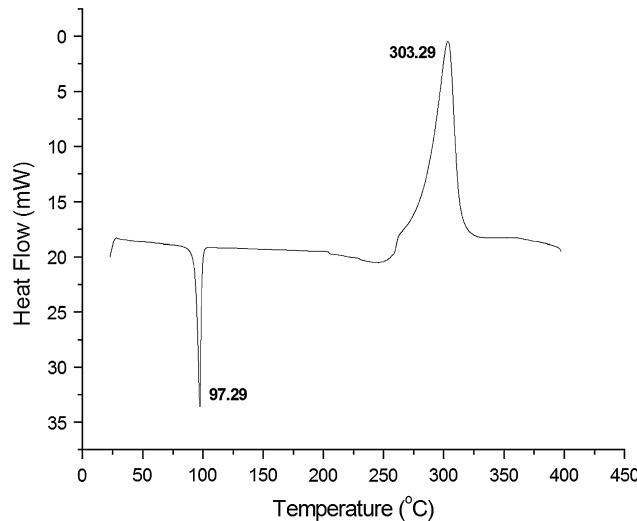
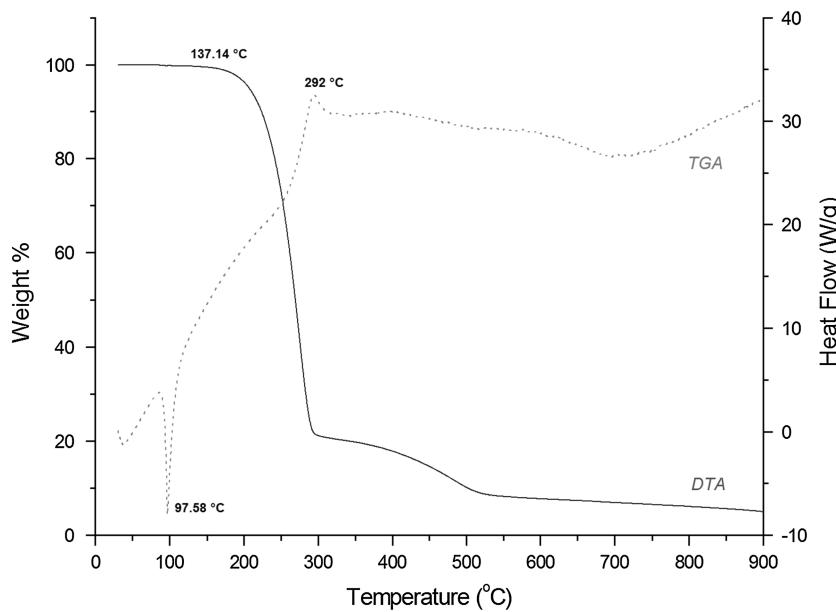


**Fig. 4** Infinite helical sheet like structure in crystal packing along c axis



corresponding to the melting point of sample, which is consistent with the uncorrected melting point taken by open capillary method and literature value [17]. The shape

of the peak suggests sharp melting and compound shows thermal stability till 137.14 °C after which decomposition starts and ca. 80 % weight loss is observed in TGA. An

**Fig. 5** TG-DTA thermogram**Fig. 6** DSC curve

exothermic peak occurs at 292.44 °C in DTA corresponding to sharp weight loss in the TGA curve. TGA curve reveals two step decomposition.

#### Differential Scanning Calorimetry

DSC data was collected on a Perkin Elmer Pyris 6 DSC. The measurement was conducted after equilibration at 25 °C, followed by a 10.00 °C min<sup>-1</sup> ramp up to 450 °C in nitrogen atmosphere. The endothermic dip at 97.29 °C is due to the melting point of the compound. There is an exothermic peak at 303.29 °C similar to DTA which is due to decomposition. DSC curve for the titled compound is shown in Fig. 6.

#### Conclusion

The synthesis of 1-(2-fluoro-4-nitrophenyl)-4-(prop-2-yn-1-yl)piperazine is reported for the first time. The formation of compound was confirmed by spectroscopy. Slow evaporation solution growth method was employed to grow single crystals of good quality for X-ray diffraction studies. The arrangement of the molecules in the crystal packing looks like parallel infinite sheets stabilized by stacking interactions of aromatic rings, C–H···O hydrogen bonds and C(aryl)–H···π interactions. Thermal studies including DSC, DTA and TGA indicated that the compound does not sublime before it melts at 97 °C.

**Acknowledgments** Satish Kumar Awasthi is thankful to University of Delhi for financial assistance and University Scientific Instrumentation Center (USIC), University of Delhi, Delhi 110007, Delhi India for analytical data. Chiranjeev Sharma is thankful to UGC for providing SRF. Gunjan Pandey is thankful, to UGC for providing JRF.

#### References

1. Tagat JR, McCombie SW, Steensma RW, Lin SI, Nazareno DV, Baroudy B, Vantuno N, Xu S, Liu J (2001) Piperazine-based CCR5 antagonists as HIV-1 inhibitors. I: 2(S)-methyl piperazine as a key pharmacophore element. *Bioorg Med Chem Lett* 11:2143–2146
2. Wang H, Xiao J, Gao D, Zhang X, Yan H, Gong Z, Sun T, Li S (2011) Pharmacophore-based design, synthesis, and biological evaluation of novel chloro-pyridazine piperazines as human rhinovirus (HRV-3) inhibitors. *Bioorg Med Chem Lett* 21:1057–1059
3. Braccio MD, Grossi G, Roma G, Signorello MG, Leoncini G (2004) Synthesis and in vitro inhibitory activity on human platelet aggregation of novel properly substituted 4-(1-piperazinyl)coumarins. *Eur J Med Chem* 39:397–409
4. Tripathi RP, Tiwari VK, Bhattacharya SM, Tyagi K, Srivastava VML, Murthy PK (2003) 7-O-[4-methyl piperazine-1-(2-acetyl)]-

- 2H-1-benzopyran-2-one: a novel antifilarial lead compound. *Acta Tropica* 87:215–224
5. Lyoqt RA, Titeler M, McKenney JD, Magee PS, Glennon RA (1986) Synthesis and evaluation of phenyl- and benzoylpiperazines as potential serotonergic agents. *J Med Chem* 29:630–634
  6. Mattson RJ, Catt JD, Keavy D, Sloan CP, Epperson J, Gao Q, Hodges DB, Iben L, Mahle CD, Ryan E, Yocca FD (2003) Indanyl piperazines as melatonergic MT<sub>2</sub> selective agents. *Bioorg Med Chem Lett* 13:1199–1202
  7. Manoury PM, Dumas AP, Naje H (1979) Synthesis and analgesic activities of some (4-substituted phenyl-1-piperazinyl)alkyl 2-amino benzoates and 2-aminonicotinates. *J Med Chem* 22:554–559
  8. Jordan S, Koprivica V, Chen R, Tottori K, Kikuchi T, Altar CA (2002) The antipsychotic aripiprazole is a potent, partial agonist at the human 5-HT<sub>1A</sub> receptor. *Eur J Pharm* 441:137–140
  9. Cusack B, Nelson A, Richelson E (1994) Binding of antidepressants to human brain receptors: focus generation compounds. *Psychopharmacology* 114:559–565
  10. Cushion MT, Walzer PD, Ashbaugh A, Rebholz S, Brubaker R, Eynde J JV, Mayence A, Huang TL (2006) In vitro selection and in vivo efficacy of piperazine- and alkanediamide-linked bis-benzamidines against *Pneumocystis pneumonia* in mice. *Antimicrob Agents Chemother* 50:2337–2343
  11. Satake N, Shibata S, Suh TK, Flores F (1984) An alpha-adrenoceptor-blocking action of SGB-483, a new piperazine antihypertensive agent in isolated vascular smooth muscles. *Blood Vessels* 21:298–305
  12. Goldman L, Williams JH (1954) Derivatives of 1-piperazine-carboxylic acid as sedatives. *J Am Chem Soc* 76:6078–6080
  13. Dixit SK, Mishra N, Sharma M, Singh S, Agarwal A, Awasthi SK, Bhasin VK (2012) Synthesis and in vitro antiplasmodial activities of fluoroquinolone analogues. *Eur J Med Chem* 51: 52–59
  14. Neupane CS, Awasthi SK (2012) Unique trifurcated hydrogen bonding in a pseudopolymorph of tricyclohexane triperoxide (TCTP) and its thermal studies. *Tetrahedron Lett* 53:6067–6070
  15. Yadav N, Dixit SK, Bhattacharya A, Mishra LC, Sharma M, Awasthi SK, Bhasin VK (2012) Antimalarial activity of newly synthesized chalcone derivatives in vitro. *Chem Biol Drug Des* 80:340–347
  16. Singh S, Singh MK, Agarwal A, Awasthi SK (2011) 2-(4-Chlorophenyl)chromen-4-one. *Acta Crystallogr Sect E* 67(Pt 12):o3163. doi:10.1107/S1600536811043832
  17. Khalaj A, Nakjiri M, Negahbani AS, Samadizadeh M, Firoozpour L, Rajabalian S, Samadi N, Faramarzi MA, Adibpour N, Shafiee A, Foroumadi A (2011) Discovery of a novel nitroimidazolyleoxazolidinone hybrid with potent anti Gram-positive activity: synthesis and antibacterial evaluation. *Eur J Med Chem* 46:65–70
  18. Padmanabhan K, Venkatesan K, Ramamurthy V (1987) Structure-reactivity correlation of photochemical reactions in organic crystals: intramolecular hydrogen abstraction in an aromatic nitro compound. *J Chem Soc Perkin Trans II*:1153–1158
  19. Viswamitra MA, Bandekar RJ Jr, Desiraju GR (1993) Evidence for O–H C and N–H C hydrogen bonding in crystalline alkynes, alkenes, and aromatics. *J Am Chem Soc* 115:4868–4869
  20. Thakur TS, Sathishkumar R, Dikundwar AG, Row TNG, Desiraju GR (2010) Third polymorph of phenylacetylene. *Cryst Growth Des* 10:4246–4249
  21. Gło'wka ML, Martynowski D, Kozłowska K (1999) Stacking of six-membered aromatic rings in crystals. *J Mol Struct* 474:81–89