



Received 18 June 2017

Accepted 10 July 2017

Edited by H. Stoeckli-Evans, University of
Neuchâtel, Switzerland**Keywords:** crystal structure; pyrene-1-carbaldehyde; *o*-phenylenediamine; benzimidazole; N—H...N hydrogen bonding; C—H... π interactions; DFT.**CCDC reference:** 1547858**Supporting information:** this article has
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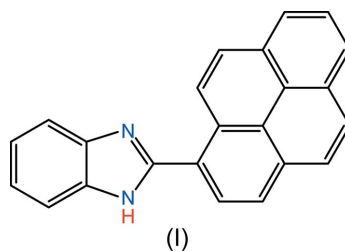
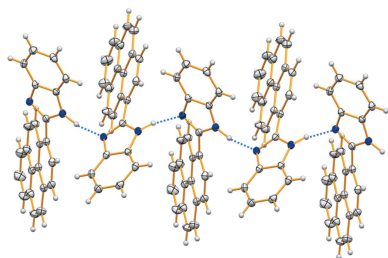
Crystal structure and DFT study of 2-(pyren-1-yl)-1*H*-benzimidazole

Md. Serajul Haque Faizi,^a Necmi Dege^b and S. Malinkin^{c*}^aDepartment of Chemistry, College of Science, Sultan Qaboos University, PO Box 36 Al-Khod 123, Muscat, Sultanate of Oman, ^bOndokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, 55139 Atakum–Samsun, Turkey, and ^cDepartment of Chemistry, National Taras Shevchenko University of Kiev, 64/13, Volodymyrska Street, City of Kyiv 01601, Ukraine. *Correspondence e-mail: malinachem88@gmail.com

In the title compound, C₂₃H₁₄N₂, (**I**), the dihedral angle between the mean planes of the pyrene and benzimidazole ring systems is 42.08 (5)°, with a bridging C—C bond length of 1.463 (3) Å. In the crystal, molecules are linked by N—H...N hydrogen bonds, forming columns propagating along the *b*-axis direction. The columns are linked *via* C—H... π interactions, forming slabs parallel to the *ab* plane. There are no significant π – π interactions present in the crystal structure. The density functional theory (DFT) optimized structure, at the B3LYP/6-311G(d,p) level, is compared with the experimentally determined solid-state structure of the title compound.

1. Chemical context

Benzimidazoles, which are analogues of imidazole contained in histidine, are an important class of biologically active compounds (Collman *et al.*, 1973). In addition, they are excellent organic ligands of many metal ions (Sundberg & Martin, 1974). The pyrene unit is one of the most commonly used fluorophores due to its strong luminescence and chemical stability (Aoki *et al.*, 1991; Nishizawa *et al.*, 1999; van der Veen *et al.*, 2000). Another interesting feature of the pyrene unit is the interaction between the pyrene aromatic rings in the crystal packing, which can permit the formation of highly ordered molecular aggregates in the solid state by architecturally controlled self-assembly (Desiraju & Gavezzotti, 1989; Munakata *et al.*, 1994). Pyrene is a commonly used fluorophore due to its unusual fluorescence properties, *viz.* intense fluorescence signals and vibronic band dependence with the media (Karpovich & Blanchard, 1995), and has been used in fluorescence sensors (Bell & Hext, 2004) and excimer formation (Lodeiro *et al.*, 2006). As a result of these particular properties and because of its chemical stability, it is also employed as a probe for solid-state studies and polymer association (Seixas de Melo *et al.*, 2003).



The title compound was prepared from an equimolar mixture of 1:1 *o*-phenylenediamine and pyrene-1-carbaldehyde. Synthesis and characterization of many benzimidazole-

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

Cg1, Cg6 and Cg7 are the centroids of rings N1/N2/C17/C18/C23, C18-C23 and N1/N2/C17-C23.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H1A\cdots N1^i$	0.94 (2)	1.92 (2)	2.838 (2)	164 (2)
$C14-H14\cdots Cg6^{ii}$	0.93	2.83	3.537 (2)	134
$C21-H21\cdots Cg1^{iii}$	0.93	2.95	3.605 (2)	129
$C21-H21\cdots Cg7^{iii}$	0.93	2.84	3.618 (2)	142

Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $x + 1, y, z$; (iii) $x - \frac{1}{2}, y, -z + \frac{1}{2}$.

ring-containing compounds have been reported (Yan *et al.*, 2009; Hallett *et al.*, 2012; Xia *et al.*, 2014; Dhanalakshmi *et al.*, 2014; Guo *et al.*, 2015; Song *et al.*, 2010), but very few compounds have been structurally characterized. Previously, Zhao *et al.* (2016) reported on the synthesis of 2-(pyren-1-yl)benzimidazole, used as a fluorescent probe for the detection of iron(III) ions in aqueous solution, but gave no structural details of the compound. The present work is part of an ongoing structural study of pyrene-ring-system derivatives (Faizi & Prisyazhnaya, 2015). The results of the calculations by density functional theory (DFT) on (**I**), carried out at the B3LYP/6-311G(d,p) level, are compared with the experimentally determined molecular structure in the solid state.

2. Structural commentary

The molecular structure of the title compound, (**I**), is illustrated in Fig. 1. The compound is nonplanar, the rotation around the bond connecting the two aromatic moieties, which is predominantly σ in character [$C16-C17 = 1.463(3) \text{\AA}$], being described by the torsion angle $N1-C17-C16-C1$ of $-39.49(10)^\circ$. The mean planes of the pyrene (atoms $C1-C16$; r.m.s. deviation = 0.038\AA) and benzimidazole ($N1/N2/C17-C23$) ring systems are inclined to one another by $42.08(5)^\circ$, reflecting the significant deviation from overall molecular planarity.

3. Supramolecular features

In the crystal of (**I**), molecules are assembled *via* $N2-H\cdots N1^i$ hydrogen bonds (Table 1) into columns propagating along the

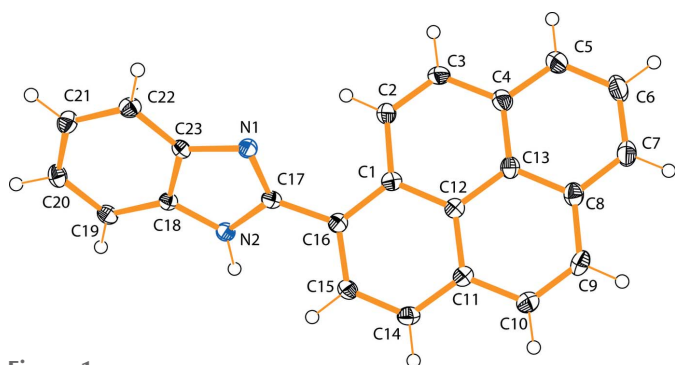


Figure 1

The molecular structure of compound (**I**), with the atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

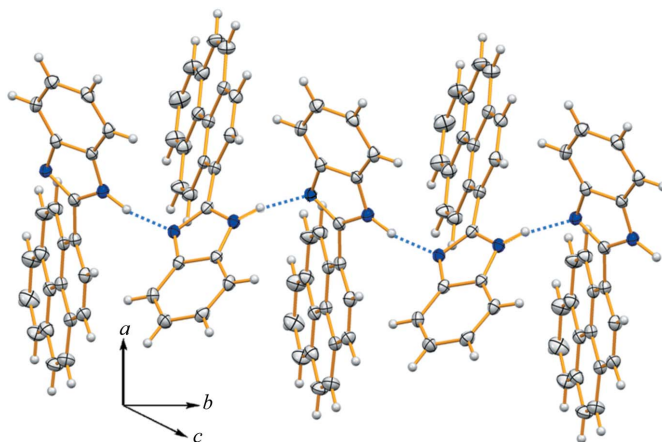


Figure 2

A view of the $N-H\cdots N$ hydrogen-bonded column (dashed lines; Table 1) in the crystal of compound (**I**), propagating along the b -axis direction.

b -axis direction (Fig. 2). The columns are linked by $C-H\cdots\pi$ interactions (Table 1), forming slabs parallel to the ab plane (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.38, last update May 2017; Groom *et al.*, 2016) gave a number of hits for similar compounds, *viz.* phenyl-2-benzimidazole derivatives (**II**) (CSD refcode FOBZUS; Li *et al.*, 2005) and (**III**) (LIYTIW; Bei *et al.*, 2000), and phenanthroimidazole derivatives (**IV**) (ERODOE; Bu *et al.*, 2003) and (**V**) (SUZHIE; Krebs *et al.*, 2001). All four organic compounds are nonplanar and have a similar $C-C$ bond length between the aromatic ring systems. In (**I**), this bond ($C16-C17$) is $1.463(3) \text{\AA}$, and the two ring systems are inclined to one

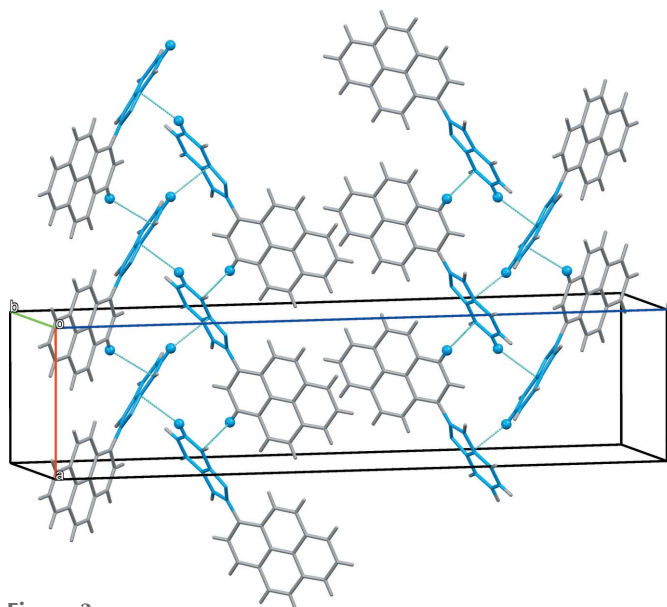


Figure 3

A view along the b axis of the crystal packing of compound (**I**). The $C-H\cdots\pi$ interactions are illustrated by dashed lines (Table 1).

Table 2

Comparison of selected geometric data for (**I**) (Å, °) from X-ray and calculated (DFT) data.

Bonds/angles	X-ray	B3LYP/6-311G(d,p)
C17–N2	1.364 (2)	1.365
C18–N2	1.376 (2)	1.375
C17–N1	1.330 (2)	1.329
C23–N1	1.389 (2)	1.389
C17–C16	1.463 (3)	1.462
C16–C17–N2	121.57 (17)	121.51
C16–C17–N1	125.73 (17)	125.82
N1–C17–N2	112.48 (17)	112.44

another by 42.08 (5)°. These values are close to those reported for compounds (**II**) (1.474 Å and 40.17°), (**III**) (1.467 Å and 31.12°) and (**V**) (1.436 and 30.12°), but the anthracene–phenanthroimidazole compound (**IV**) has a larger deviation from planarity, with the two aromatic ring systems being

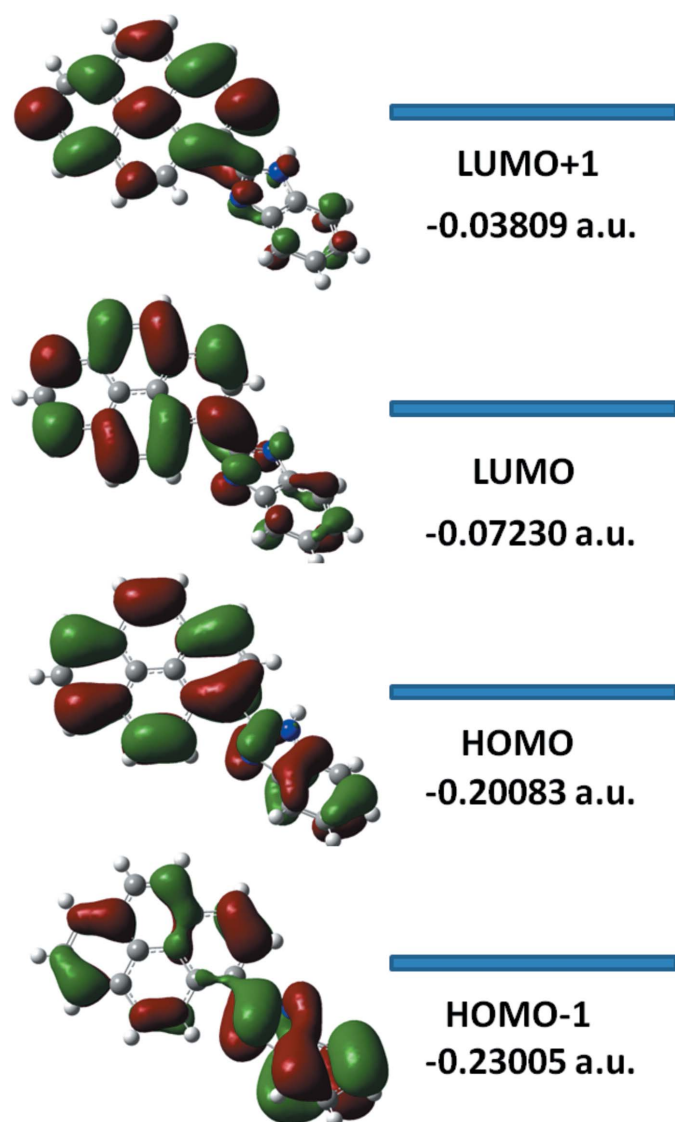


Figure 4
Electron distribution of the HOMO-1, HOMO, LUMO and LUMO+1 energy levels for compound (**I**).

almost perpendicular to one another (1.488 Å and 76.54°) due to significant steric hindrance of the anthracene moiety. Two other compounds are worth mentioning, *viz.* 9-(1*H*-benzimidazol-2-yl)-2,3,6,7-tetrahydro-1*H*,5*H*-pyrido[3,2,1-*ij*]quinoline (**VI**) (TAQHUR; Gonzalez & Unnamatla, 2017) and 2-(pyren-1-yl)-1*H*-phenanthro[9,10-*d*]imidazole unknown solvate (**VII**) (KUFLOO; Subeesh *et al.*, 2015). In (**VI**), the mean plane of the pyridoquinoline moiety is inclined to the benzimidazole ring system by 37.94 (10)° and the bridging C–C bond is 1.467 (3) Å, similar to the situation in (**I**). In (**VII**), the mean plane of the pyrene ring system is inclined to the phenanthroimidazole mean plane by 63.37 (6)° and the bridging C–C bond is 1.463 (5) Å. As in (**IV**), this large dihedral angle is due to steric hinderance.

5. DFT study

The DFT quantum-chemical calculations were performed at the B3LYP/6-311G(d,p) level (Becke, 1993), as implemented in *GAUSSIAN09* (Frisch *et al.*, 2009). DFT structure optimization of (**I**) was performed starting from the X-ray geometry and the values compared with experimental values (see Table 2). From these results we can conclude that basis set 6-311G(d,p) is well suited in its approach to the experimental data.

The DFT study of (**I**) shows that the HOMO and LUMO are localized in the plane extending from the whole pyrene ring to the benzimidazole ring. The electron distribution of the HOMO-1, HOMO, LUMO and the LUMO+1 energy levels are shown in Fig. 4. The molecular orbital of HOMO contains both σ and π character, whereas HOMO-1 is dominated by orbital density. The LUMO is mainly composed of density, while LUMO+1 has both σ and π character and electronic density. The HOMO–LUMO gap was found to be 0.273 a.u. and the frontier molecular orbital energies, E_{HOMO} and E_{LUMO} , were -0.20083 and -0.07230 a.u., respectively.

6. Synthesis and crystallization

Pyrene-1-carbaldehyde (0.2306 g, 1.0 mmol) was added to a 50 ml round-bottomed flask containing 10 ml of CH_2Cl_2 . Then a 10 ml CH_2Cl_2 solution containing 0.1080 g (1.0 mmol) *o*-phenylenediamine was added dropwise over a period of 30 min with stirring. The mixture was stirred at room temperature for 48 h. The solvent was then evaporated and the residue purified by aluminium oxide gel-column chromatography using CH_2Cl_2 as the eluent to obtain a pale-yellow powder of (**I**) (yield 0.2311 g, 72.6%). Colourless prismatic crystals were obtained by slow evaporation of a solution of (**I**) from methanol.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The N-bound H atoms were located in a difference Fourier map and refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The C-bound H atoms were included in calculated

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₂₃ H ₁₄ N ₂
<i>M_r</i>	318.36
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	273
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.7344 (8), 9.5967 (9), 36.410 (3)
<i>V</i> (Å ³)	3052.0 (5)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm ⁻¹)	0.08
Crystal size (mm)	0.65 × 0.43 × 0.32
Data collection	
Diffractometer	Bruker APEXII CCD area detector
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	36046, 2986, 1951
<i>R</i> _{int}	0.103
(sin θ/λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.049, 0.113, 1.03
No. of reflections	2986
No. of parameters	230
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.19, -0.26

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2005), *SHELXT2014* (Sheldrick, 2015a), *SHELXTL* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

positions and refined as riding, with C–H = 0.93–0.96 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

The authors are grateful to the Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, Samsun, Turkey, for X-ray data collection and the Department of Chemistry, National Taras Shevchenko University of Kiev, Kyiv, Ukraine.

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supporting information

Acta Cryst. (2017). E73, 1180-1183 [https://doi.org/10.1107/S2056989017010271]

Crystal structure and DFT study of 2-(pyren-1-yl)-1*H*-benzimidazole

Md. Serajul Haque Faizi, Necmi Dege and S. Malinkin

Computing details

Data collection: *APEX2* (Bruker, 2005); data reduction: *SAINTE* (Bruker, 2005); program(s) used to solve structure: *SHELXT2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

2-(Pyren-1-yl)-1*H*-benzimidazole

Crystal data

$C_{23}H_{14}N_2$

$M_r = 318.36$

Orthorhombic, *Pbca*

$a = 8.7344$ (8) Å

$b = 9.5967$ (9) Å

$c = 36.410$ (3) Å

$V = 3052.0$ (5) Å³

$Z = 8$

$F(000) = 1328$

$D_x = 1.386$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 1528 reflections

$\theta = 2.4$ – 16.1°

$\mu = 0.08$ mm⁻¹

$T = 273$ K

Prism, colorless

$0.65 \times 0.43 \times 0.32$ mm

Data collection

Bruker APEXII CCD area detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

phi and ω scans

36046 measured reflections

2986 independent reflections

1951 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.103$

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.6^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -44 \rightarrow 44$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.113$

$S = 1.03$

2986 reflections

230 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 1.2809P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.19$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.15929 (18)	0.66443 (16)	0.32741 (4)	0.0190 (4)
N2	0.21591 (19)	0.89171 (17)	0.32393 (5)	0.0195 (4)
C23	0.0470 (2)	0.73209 (19)	0.30713 (5)	0.0176 (5)
C17	0.2581 (2)	0.7637 (2)	0.33673 (5)	0.0190 (5)
C16	0.4042 (2)	0.74213 (19)	0.35556 (5)	0.0195 (5)
C18	0.0808 (2)	0.8748 (2)	0.30499 (5)	0.0179 (4)
C1	0.4229 (2)	0.6448 (2)	0.38432 (5)	0.0193 (5)
C12	0.5724 (2)	0.6212 (2)	0.39850 (5)	0.0199 (5)
C11	0.6999 (2)	0.6952 (2)	0.38411 (5)	0.0210 (5)
C19	-0.0099 (2)	0.9680 (2)	0.28557 (5)	0.0214 (5)
H19	0.012157	1.062811	0.284937	0.026*
C20	-0.1341 (2)	0.9132 (2)	0.26728 (5)	0.0235 (5)
H20	-0.195476	0.971887	0.253275	0.028*
C13	0.5956 (2)	0.5241 (2)	0.42759 (5)	0.0220 (5)
C2	0.2978 (2)	0.5706 (2)	0.40072 (6)	0.0235 (5)
H2	0.198943	0.585875	0.392152	0.028*
C8	0.7452 (2)	0.4990 (2)	0.44151 (5)	0.0252 (5)
C14	0.6749 (2)	0.7950 (2)	0.35696 (6)	0.0239 (5)
H14	0.756769	0.847263	0.348192	0.029*
C4	0.4691 (2)	0.4519 (2)	0.44303 (6)	0.0253 (5)
C15	0.5309 (2)	0.8170 (2)	0.34299 (6)	0.0231 (5)
H15	0.517365	0.883532	0.324701	0.028*
C22	-0.0814 (2)	0.6796 (2)	0.28931 (5)	0.0224 (5)
H22	-0.106657	0.585627	0.290863	0.027*
C21	-0.1703 (2)	0.7709 (2)	0.26926 (5)	0.0247 (5)
H21	-0.255742	0.737591	0.256826	0.030*
C10	0.8497 (2)	0.6653 (2)	0.39798 (6)	0.0273 (5)
H10	0.933899	0.711258	0.388120	0.033*
C9	0.8707 (2)	0.5716 (2)	0.42512 (6)	0.0292 (5)
H9	0.969483	0.553670	0.433385	0.035*
C3	0.3207 (2)	0.4788 (2)	0.42841 (6)	0.0271 (5)
H3	0.236939	0.431824	0.438185	0.033*
C7	0.7635 (3)	0.4060 (2)	0.47055 (6)	0.0311 (6)
H7	0.860961	0.389193	0.479795	0.037*
C5	0.4941 (3)	0.3609 (2)	0.47218 (6)	0.0318 (6)
H5	0.411550	0.314383	0.482643	0.038*
C6	0.6397 (3)	0.3386 (2)	0.48582 (6)	0.0357 (6)
H6	0.654109	0.277746	0.505401	0.043*
H1A	0.271 (2)	0.975 (2)	0.3280 (6)	0.033 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0191 (9)	0.0153 (9)	0.0225 (9)	0.0003 (7)	-0.0016 (8)	0.0003 (8)
N2	0.0203 (10)	0.0129 (9)	0.0253 (9)	-0.0010 (8)	-0.0014 (8)	0.0010 (7)
C23	0.0207 (11)	0.0152 (10)	0.0170 (10)	0.0012 (8)	0.0014 (9)	0.0013 (8)
C17	0.0198 (11)	0.0168 (11)	0.0205 (10)	0.0007 (9)	0.0039 (10)	0.0006 (8)
C16	0.0200 (11)	0.0158 (10)	0.0227 (11)	0.0009 (9)	0.0000 (10)	-0.0016 (8)
C18	0.0177 (11)	0.0180 (10)	0.0181 (10)	0.0013 (8)	0.0016 (9)	-0.0006 (8)
C1	0.0201 (11)	0.0167 (11)	0.0210 (11)	0.0009 (9)	0.0014 (9)	-0.0029 (9)
C12	0.0208 (11)	0.0187 (11)	0.0202 (10)	0.0009 (9)	0.0008 (9)	-0.0029 (9)
C11	0.0201 (11)	0.0205 (11)	0.0224 (11)	0.0009 (9)	0.0002 (9)	-0.0035 (9)
C19	0.0258 (12)	0.0151 (10)	0.0234 (11)	0.0019 (9)	0.0021 (10)	0.0015 (9)
C20	0.0254 (12)	0.0232 (12)	0.0221 (11)	0.0076 (9)	-0.0011 (10)	0.0011 (9)
C13	0.0228 (12)	0.0220 (11)	0.0213 (11)	0.0038 (9)	-0.0002 (10)	-0.0012 (9)
C2	0.0200 (12)	0.0235 (11)	0.0270 (12)	0.0024 (9)	-0.0002 (10)	0.0027 (10)
C8	0.0246 (12)	0.0265 (12)	0.0246 (11)	0.0052 (9)	-0.0009 (10)	0.0005 (9)
C14	0.0212 (12)	0.0218 (11)	0.0288 (12)	-0.0035 (9)	0.0036 (10)	0.0010 (9)
C4	0.0260 (12)	0.0237 (12)	0.0263 (12)	0.0027 (10)	0.0006 (10)	0.0027 (9)
C15	0.0260 (12)	0.0174 (11)	0.0259 (11)	0.0005 (9)	-0.0005 (10)	0.0036 (9)
C22	0.0253 (12)	0.0154 (11)	0.0267 (11)	-0.0014 (9)	-0.0005 (10)	-0.0022 (9)
C21	0.0240 (12)	0.0246 (12)	0.0256 (12)	0.0009 (9)	-0.0043 (10)	-0.0032 (9)
C10	0.0208 (12)	0.0316 (13)	0.0296 (12)	-0.0013 (10)	0.0027 (10)	0.0018 (10)
C9	0.0183 (12)	0.0361 (14)	0.0333 (13)	0.0056 (10)	-0.0041 (10)	-0.0008 (11)
C3	0.0209 (12)	0.0287 (12)	0.0317 (12)	-0.0023 (10)	0.0046 (10)	0.0075 (10)
C7	0.0259 (13)	0.0351 (13)	0.0325 (12)	0.0066 (10)	-0.0054 (11)	0.0050 (10)
C5	0.0289 (13)	0.0341 (14)	0.0326 (13)	0.0015 (11)	0.0033 (11)	0.0102 (10)
C6	0.0367 (14)	0.0382 (14)	0.0322 (13)	0.0097 (11)	-0.0022 (12)	0.0143 (11)

Geometric parameters (Å, °)

N1—C17	1.330 (2)	C13—C8	1.423 (3)
N1—C23	1.389 (2)	C2—C3	1.354 (3)
N2—C17	1.364 (2)	C2—H2	0.9300
N2—C18	1.376 (2)	C8—C7	1.392 (3)
N2—H1A	0.94 (2)	C8—C9	1.429 (3)
C23—C22	1.390 (3)	C14—C15	1.373 (3)
C23—C18	1.403 (3)	C14—H14	0.9300
C17—C16	1.463 (3)	C4—C5	1.391 (3)
C16—C15	1.397 (3)	C4—C3	1.425 (3)
C16—C1	1.412 (3)	C15—H15	0.9300
C18—C19	1.389 (3)	C22—C21	1.380 (3)
C1—C12	1.422 (3)	C22—H22	0.9300
C1—C2	1.434 (3)	C21—H21	0.9300
C12—C11	1.421 (3)	C10—C9	1.349 (3)
C12—C13	1.426 (3)	C10—H10	0.9300
C11—C14	1.393 (3)	C9—H9	0.9300
C11—C10	1.431 (3)	C3—H3	0.9300

C19—C20	1.377 (3)	C7—C6	1.378 (3)
C19—H19	0.9300	C7—H7	0.9300
C20—C21	1.403 (3)	C5—C6	1.381 (3)
C20—H20	0.9300	C5—H5	0.9300
C13—C4	1.420 (3)	C6—H6	0.9300
C17—N1—C23	105.01 (16)	C7—C8—C13	118.9 (2)
C17—N2—C18	107.25 (16)	C7—C8—C9	122.8 (2)
C17—N2—H1A	124.7 (13)	C13—C8—C9	118.26 (18)
C18—N2—H1A	128.1 (13)	C15—C14—C11	120.81 (19)
N1—C23—C22	130.42 (18)	C15—C14—H14	119.6
N1—C23—C18	109.72 (17)	C11—C14—H14	119.6
C22—C23—C18	119.84 (18)	C5—C4—C13	119.1 (2)
N1—C17—N2	112.48 (17)	C5—C4—C3	122.8 (2)
N1—C17—C16	125.73 (17)	C13—C4—C3	118.12 (18)
N2—C17—C16	121.57 (17)	C14—C15—C16	121.67 (19)
C15—C16—C1	119.46 (18)	C14—C15—H15	119.2
C15—C16—C17	117.66 (17)	C16—C15—H15	119.2
C1—C16—C17	122.80 (18)	C21—C22—C23	118.06 (19)
N2—C18—C19	131.90 (18)	C21—C22—H22	121.0
N2—C18—C23	105.54 (16)	C23—C22—H22	121.0
C19—C18—C23	122.51 (18)	C22—C21—C20	121.24 (19)
C16—C1—C12	118.71 (18)	C22—C21—H21	119.4
C16—C1—C2	123.31 (19)	C20—C21—H21	119.4
C12—C1—C2	117.96 (18)	C9—C10—C11	121.1 (2)
C11—C12—C1	120.40 (18)	C9—C10—H10	119.4
C11—C12—C13	119.29 (18)	C11—C10—H10	119.4
C1—C12—C13	120.30 (18)	C10—C9—C8	121.8 (2)
C14—C11—C12	118.83 (18)	C10—C9—H9	119.1
C14—C11—C10	122.10 (19)	C8—C9—H9	119.1
C12—C11—C10	119.07 (18)	C2—C3—C4	122.0 (2)
C20—C19—C18	116.68 (19)	C2—C3—H3	119.0
C20—C19—H19	121.7	C4—C3—H3	119.0
C18—C19—H19	121.7	C6—C7—C8	121.2 (2)
C19—C20—C21	121.62 (19)	C6—C7—H7	119.4
C19—C20—H20	119.2	C8—C7—H7	119.4
C21—C20—H20	119.2	C6—C5—C4	121.1 (2)
C4—C13—C8	119.43 (18)	C6—C5—H5	119.5
C4—C13—C12	120.17 (18)	C4—C5—H5	119.5
C8—C13—C12	120.40 (19)	C7—C6—C5	120.3 (2)
C3—C2—C1	121.41 (19)	C7—C6—H6	119.9
C3—C2—H2	119.3	C5—C6—H6	119.9
C1—C2—H2	119.3		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1, Cg6 and Cg7 are the centroids of rings N1/N2/C17/C18/C23, C18-C23 and N1/N2/C17-C23.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H1A \cdots N1 ⁱ	0.94 (2)	1.92 (2)	2.838 (2)	164 (2)
C14—H14 \cdots Cg6 ⁱⁱ	0.93	2.83	3.537 (2)	134
C21—H21 \cdots Cg1 ⁱⁱⁱ	0.93	2.95	3.605 (2)	129
C21—H21 \cdots Cg7 ⁱⁱⁱ	0.93	2.84	3.618 (2)	142

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