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***N,N*-Dimethyl-4-(pyren-1-yl)aniline**Sreevidya Thekku Veedu,^{a,b*} Mirko Scholz,^b Reza Kia,^{a,b}
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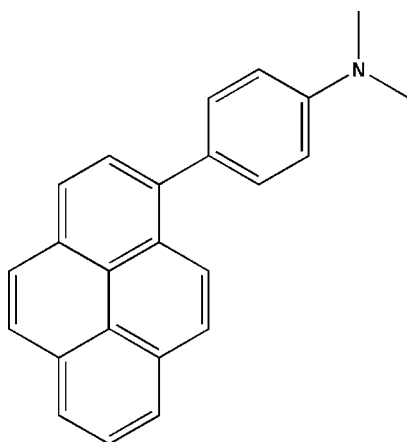
Received 29 November 2013; accepted 2 December 2013

Key indicators: single-crystal synchrotron study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.047; wR factor = 0.135; data-to-parameter ratio = 25.8.

In the title compound, $\text{C}_{24}\text{H}_{19}\text{N}$, the dimethylamino group is inclined to the benzene ring by $2.81(9)^\circ$. Their mean plane makes a dihedral angle of $64.12(2)^\circ$ with the mean plane of the pyrene ring system [r.m.s. deviation = $0.031(1)$ Å]. In the crystal, molecules are linked *via* $\text{C}-\text{H}\cdots\pi$ interactions, which connect neighbouring molecules into columns along the c axis.

Related literature

For charge transfer involving donor and acceptor molecules, see: Wasielewski (1992); Willemse *et al.* (2000). For a related structure, *N,N*-Diphenyl-4-(pyren-1-yl)aniline, see: Wang *et al.* (2010). For the synthesis of the title compound, see: Dewar & Mole (1956); Norman *et al.* (1958). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{24}\text{H}_{19}\text{N}$ $M_r = 321.40$ Monoclinic, $P2_1/c$
 $a = 6.1270(12)$ Å
 $b = 30.686(6)$ Å
 $c = 9.478(3)$ Å
 $\beta = 113.35(2)^\circ$
 $V = 1636.0(8)$ Å³ $Z = 4$
Synchrotron radiation
 $\lambda = 0.600$ Å
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.15 \times 0.10$ mm

Data collection

Huber diffractometer with a Mar
CCD detector
Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)
 $T_{\min} = 0.978$, $T_{\max} = 0.993$ 47866 measured reflections
5872 independent reflections
4806 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.135$
 $S = 1.08$
5872 reflections228 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 Cg1 , Cg2 , Cg3 , Cg4 and Cg5 are the centroids of the $\text{C1}-\text{C6}$, $\text{C7}-\text{C10}/\text{C19}/\text{C20}$, $\text{C10}-\text{C13}/\text{C18}/\text{C19}$, $\text{C13}-\text{C18}$ and $\text{C17}-\text{C22}$ rings, respectively.

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C2}-\text{H2}\cdots\text{Cg2}^{\text{i}}$ | 0.95 | 2.93 | 3.6043 (15) | 129 |
| $\text{C6}-\text{H6}\cdots\text{Cg5}^{\text{ii}}$ | 0.95 | 2.90 | 3.6495 (15) | 137 |
| $\text{C22}-\text{H22}\cdots\text{Cg1}^{\text{iii}}$ | 0.95 | 2.68 | 3.5499 (15) | 152 |
| $\text{C23}-\text{H52A}\cdots\text{Cg3}^{\text{i}}$ | 0.98 | 2.74 | 3.5994 (15) | 147 |
| $\text{C24}-\text{H52E}\cdots\text{Cg4}^{\text{ii}}$ | 0.98 | 2.77 | 3.5284 (15) | 135 |

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

Data collection: *XDS* (Kabsch, 1993); cell refinement: *XDS*; data reduction: *XDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2671).

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supplementary materials

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***N,N*-Dimethyl-4-(pyren-1-yl)aniline**

Sreevidya Thekku Veedu, Mirko Scholz, Reza Kia, Carsten Paulmann and Simone Techert

1. Comment

Electron donor acceptor molecules play an important role in the understanding of charge transfer processes. In the past decades, in order to gain more insight into electron transfer processes, extensive studies have been carried out on the optical behavior of systems consisting of donor acceptor groups linked by different bridges (Wasielowski, 1992; Willemse *et al.*, 2000). These molecules are also ideal systems for studying the solvation dynamics and also for the demonstration of non-linear optical properties. Pyrene-*N,N*-dimethylaniline (PyDMA), is a compound in which the electron donor *N,N*-dimethylaniline (DMA) is covalently linked to the electron acceptor pyrene. Due to the lack of an extended bridge between the donor and acceptor in PyDMA, the physical characteristics of these groups strongly influence the electron transfer mechanism. This leads to a very unusual absorption and emission spectra in the optical regime and because of this PyDMA is considered to be a molecular diode where electron donor and electron acceptor moieties are twisted against each other modulating the electron charge transfer processes.

The title compound, Fig. 1, is a pyrene derivative. The bond lengths (Allen *et al.*, 1987) and angles are within the normal ranges and are comparable to those reported for a similar structure, *N,N*-Diphenyl-4-(pyren-1-yl)aniline (Wang *et al.*, 2010). The dimethylamine group and the benzene ring are almost coplanar (dihedral angle = 2.81 (9) °) and their mean plane makes a dihedral angle of 64.12 (2) ° with the pyrene ring system [r.m.s.d. = 0.031 (1) Å].

In the crystal, packing is stabilized by C—H... π interactions (Table 1). The interaction C23—H52A...Cg3ⁱ (see Table 1; Cg3 is the centroid of the C10-C13/C18/C19 ring) connects neighbouring molecules into columns along the *c*-axis (Fig. 2).

2. Experimental

Commercially available 1-aminopyrene after diazotization reaction was coupled with *N,N*-dimethylaniline according to the previously reported procedure (Dewar & Mole, 1956; Norman *et al.*, 1958). The crude product was then purified on an aluminium oxide column with a mixture of cyclohexane/toluene as eluent and applying HPLC. Block-like colourless crystals of the title compound were obtained by crystallization from ethyl acetate/diethyl ether (2:1) by slow evaporation.

3. Refinement

The C-bound H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.95 and 0.98 Å for CH and CH₃ H-atoms, respectively, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and = $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

Computing details

Data collection: XDS (Kabsch, 1993); cell refinement: XDS (Kabsch, 1993); data reduction: XDS (Kabsch, 1993); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

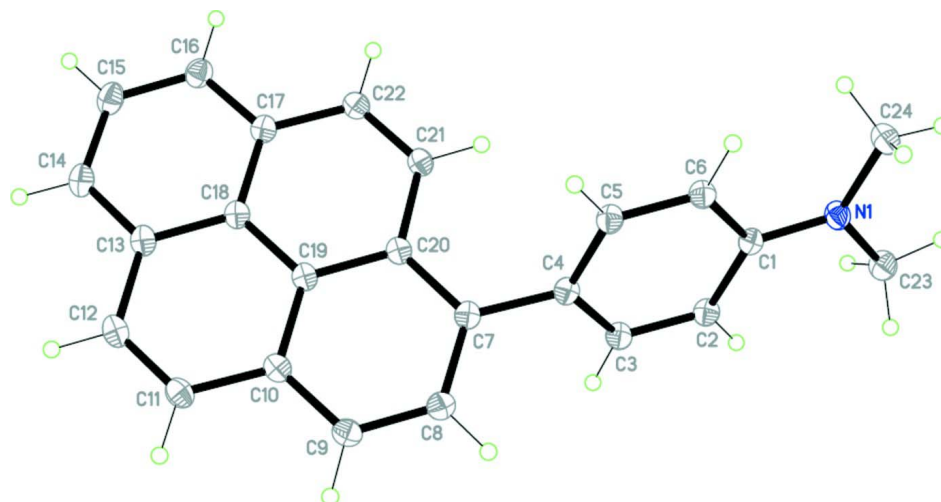


Figure 1

The molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

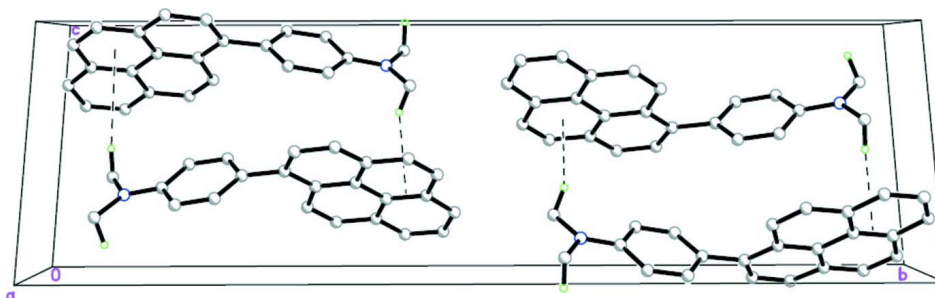


Figure 2

The crystal packing of the title compound, viewed along the *a* axis, showing molecules linked by C—H... π interactions (dashed lines; see Table 1 for details).

N,N-Dimethyl-4-(pyren-1-yl)aniline

Crystal data

$C_{24}H_{19}N$

$M_r = 321.40$

Monoclinic, $P2_1/c$

$a = 6.1270$ (12) Å

$b = 30.686$ (6) Å

$c = 9.478$ (3) Å

$\beta = 113.35$ (2)°

$V = 1636.0$ (8) Å³

$Z = 4$

$F(000) = 680$

$D_x = 1.305$ Mg m⁻³

Synchrotron radiation, $\lambda = 0.600$ Å

Cell parameters from 2549 reflections

$\theta = 2.5$ – 26.7 °

$\mu = 0.08$ mm⁻¹

$T = 100$ K

Block, colourless

$0.30 \times 0.15 \times 0.10$ mm

Data collection

Huber

diffractometer with a Mar CCD detector

Radiation source: synchrotron

φ and ω scan

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.978$, $T_{\max} = 0.993$

47866 measured reflections

5872 independent reflections

4806 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$
 $\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.1^\circ$

$h = -8 \rightarrow 9$
 $k = -44 \rightarrow 45$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.135$
 $S = 1.08$
 5872 reflections
 228 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.2446P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 | 0.83448 (13) | 0.39409 (2) | 0.82389 (9) | 0.0218 (2) |
| C1 | 0.89994 (14) | 0.35082 (3) | 0.85268 (9) | 0.0180 (2) |
| C2 | 1.05726 (15) | 0.33134 (3) | 0.79588 (10) | 0.0198 (2) |
| C3 | 1.11516 (15) | 0.28751 (3) | 0.82171 (10) | 0.0199 (2) |
| C4 | 1.01916 (14) | 0.26098 (3) | 0.90243 (9) | 0.0187 (2) |
| C5 | 0.86753 (15) | 0.28065 (3) | 0.96166 (10) | 0.0201 (2) |
| C6 | 0.80935 (15) | 0.32448 (3) | 0.93886 (10) | 0.0197 (2) |
| C7 | 1.07388 (14) | 0.21366 (3) | 0.92100 (9) | 0.0184 (2) |
| C8 | 1.30833 (15) | 0.19960 (3) | 0.99985 (10) | 0.0207 (2) |
| C9 | 1.36781 (15) | 0.15583 (3) | 1.01804 (10) | 0.0214 (2) |
| C10 | 1.19330 (14) | 0.12377 (3) | 0.95599 (9) | 0.0193 (2) |
| C11 | 1.24827 (15) | 0.07810 (3) | 0.97107 (10) | 0.0222 (2) |
| C12 | 1.07813 (16) | 0.04746 (3) | 0.90639 (10) | 0.0226 (2) |
| C13 | 0.83518 (15) | 0.05968 (3) | 0.81869 (10) | 0.0207 (2) |
| C14 | 0.65740 (17) | 0.02878 (3) | 0.74593 (11) | 0.0250 (2) |
| C15 | 0.42488 (17) | 0.04181 (3) | 0.66041 (11) | 0.0266 (2) |
| C16 | 0.36320 (16) | 0.08558 (3) | 0.64636 (10) | 0.0236 (2) |
| C17 | 0.53509 (15) | 0.11768 (3) | 0.71636 (9) | 0.0194 (2) |
| C18 | 0.77440 (14) | 0.10477 (3) | 0.80332 (9) | 0.0184 (2) |
| C19 | 0.95341 (14) | 0.13704 (3) | 0.87271 (9) | 0.0176 (2) |
| C20 | 0.89286 (14) | 0.18211 (3) | 0.85573 (9) | 0.0176 (2) |
| C21 | 0.64894 (14) | 0.19381 (3) | 0.76703 (10) | 0.0193 (2) |
| C22 | 0.47894 (14) | 0.16319 (3) | 0.70109 (10) | 0.0204 (2) |
| C23 | 0.94074 (16) | 0.42139 (3) | 0.74417 (11) | 0.0248 (2) |
| C24 | 0.67405 (16) | 0.41312 (3) | 0.88441 (11) | 0.0249 (2) |
| H2 | 1.12420 | 0.34840 | 0.73940 | 0.0240* |
| H3 | 1.22310 | 0.27520 | 0.78340 | 0.0240* |

| | | | | |
|------|---------|----------|---------|---------|
| H5 | 0.80260 | 0.26350 | 1.01910 | 0.0240* |
| H6 | 0.70730 | 0.33690 | 0.98170 | 0.0240* |
| H8 | 1.43040 | 0.22070 | 1.04220 | 0.0250* |
| H9 | 1.52870 | 0.14750 | 1.07320 | 0.0260* |
| H11 | 1.40770 | 0.06910 | 1.02770 | 0.0270* |
| H12 | 1.12010 | 0.01750 | 0.91920 | 0.0270* |
| H14 | 0.69630 | -0.00130 | 0.75520 | 0.0300* |
| H15 | 0.30680 | 0.02050 | 0.61100 | 0.0320* |
| H16 | 0.20290 | 0.09390 | 0.58870 | 0.0280* |
| H21 | 0.60590 | 0.22370 | 0.75430 | 0.0230* |
| H22 | 0.31970 | 0.17210 | 0.64370 | 0.0240* |
| H52A | 0.90310 | 0.40970 | 0.64090 | 0.0370* |
| H52B | 1.11360 | 0.42200 | 0.80130 | 0.0370* |
| H52C | 0.87760 | 0.45110 | 0.73620 | 0.0370* |
| H52D | 0.63160 | 0.44270 | 0.84360 | 0.0370* |
| H52E | 0.75170 | 0.41430 | 0.99680 | 0.0370* |
| H52F | 0.52990 | 0.39530 | 0.85400 | 0.0370* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|------------|-------------|
| N1 | 0.0259 (3) | 0.0181 (3) | 0.0254 (4) | 0.0010 (3) | 0.0143 (3) | 0.0023 (3) |
| C1 | 0.0195 (3) | 0.0180 (4) | 0.0158 (3) | -0.0010 (3) | 0.0064 (3) | -0.0002 (3) |
| C2 | 0.0232 (3) | 0.0206 (4) | 0.0181 (3) | -0.0012 (3) | 0.0109 (3) | 0.0008 (3) |
| C3 | 0.0229 (3) | 0.0208 (4) | 0.0188 (4) | -0.0002 (3) | 0.0112 (3) | -0.0007 (3) |
| C4 | 0.0211 (3) | 0.0185 (4) | 0.0169 (3) | -0.0010 (3) | 0.0080 (3) | -0.0008 (3) |
| C5 | 0.0242 (4) | 0.0194 (4) | 0.0198 (4) | -0.0015 (3) | 0.0121 (3) | 0.0004 (3) |
| C6 | 0.0226 (3) | 0.0196 (4) | 0.0197 (4) | 0.0001 (3) | 0.0114 (3) | 0.0000 (3) |
| C7 | 0.0219 (3) | 0.0189 (4) | 0.0159 (3) | -0.0004 (3) | 0.0092 (3) | -0.0006 (3) |
| C8 | 0.0210 (3) | 0.0224 (4) | 0.0186 (4) | -0.0012 (3) | 0.0079 (3) | -0.0019 (3) |
| C9 | 0.0204 (3) | 0.0245 (4) | 0.0186 (3) | 0.0019 (3) | 0.0070 (3) | -0.0001 (3) |
| C10 | 0.0218 (3) | 0.0210 (4) | 0.0155 (3) | 0.0023 (3) | 0.0077 (3) | 0.0008 (3) |
| C11 | 0.0244 (4) | 0.0226 (4) | 0.0194 (4) | 0.0045 (3) | 0.0085 (3) | 0.0018 (3) |
| C12 | 0.0293 (4) | 0.0192 (4) | 0.0201 (4) | 0.0043 (3) | 0.0107 (3) | 0.0016 (3) |
| C13 | 0.0271 (4) | 0.0188 (4) | 0.0168 (3) | 0.0007 (3) | 0.0092 (3) | 0.0004 (3) |
| C14 | 0.0319 (4) | 0.0184 (4) | 0.0239 (4) | -0.0022 (3) | 0.0103 (3) | -0.0006 (3) |
| C15 | 0.0300 (4) | 0.0219 (4) | 0.0251 (4) | -0.0054 (3) | 0.0079 (3) | -0.0012 (3) |
| C16 | 0.0239 (4) | 0.0233 (4) | 0.0215 (4) | -0.0025 (3) | 0.0067 (3) | 0.0001 (3) |
| C17 | 0.0224 (4) | 0.0201 (4) | 0.0157 (3) | -0.0006 (3) | 0.0076 (3) | 0.0005 (3) |
| C18 | 0.0225 (3) | 0.0185 (4) | 0.0145 (3) | 0.0001 (3) | 0.0078 (3) | 0.0003 (3) |
| C19 | 0.0216 (3) | 0.0180 (4) | 0.0139 (3) | 0.0011 (3) | 0.0079 (3) | 0.0002 (3) |
| C20 | 0.0213 (3) | 0.0183 (4) | 0.0143 (3) | 0.0009 (3) | 0.0082 (3) | 0.0005 (3) |
| C21 | 0.0219 (3) | 0.0189 (4) | 0.0170 (3) | 0.0023 (3) | 0.0077 (3) | 0.0014 (3) |
| C22 | 0.0210 (3) | 0.0218 (4) | 0.0177 (3) | 0.0016 (3) | 0.0070 (3) | 0.0014 (3) |
| C23 | 0.0285 (4) | 0.0222 (4) | 0.0263 (4) | 0.0006 (3) | 0.0138 (3) | 0.0056 (3) |
| C24 | 0.0290 (4) | 0.0222 (4) | 0.0269 (4) | 0.0045 (3) | 0.0148 (3) | 0.0023 (3) |

Geometric parameters (Å, °)

| | | | |
|-------------|-------------|-------------|-------------|
| N1—C1 | 1.3826 (12) | C17—C22 | 1.4318 (14) |
| N1—C23 | 1.4445 (13) | C18—C19 | 1.4298 (13) |
| N1—C24 | 1.4433 (14) | C19—C20 | 1.4244 (14) |
| C1—C2 | 1.4098 (14) | C20—C21 | 1.4399 (14) |
| C1—C6 | 1.4099 (14) | C21—C22 | 1.3573 (14) |
| C2—C3 | 1.3878 (14) | C2—H2 | 0.9500 |
| C3—C4 | 1.3967 (14) | C3—H3 | 0.9500 |
| C4—C5 | 1.3986 (14) | C5—H5 | 0.9500 |
| C4—C7 | 1.4850 (14) | C6—H6 | 0.9500 |
| C5—C6 | 1.3862 (14) | C8—H8 | 0.9500 |
| C7—C8 | 1.3990 (14) | C9—H9 | 0.9500 |
| C7—C20 | 1.4164 (14) | C11—H11 | 0.9500 |
| C8—C9 | 1.3845 (14) | C12—H12 | 0.9500 |
| C9—C10 | 1.3995 (14) | C14—H14 | 0.9500 |
| C10—C11 | 1.4352 (14) | C15—H15 | 0.9500 |
| C10—C19 | 1.4246 (13) | C16—H16 | 0.9500 |
| C11—C12 | 1.3565 (14) | C21—H21 | 0.9500 |
| C12—C13 | 1.4375 (15) | C22—H22 | 0.9500 |
| C13—C14 | 1.4020 (14) | C23—H52A | 0.9800 |
| C13—C18 | 1.4253 (14) | C23—H52B | 0.9800 |
| C14—C15 | 1.3897 (16) | C23—H52C | 0.9800 |
| C15—C16 | 1.3873 (14) | C24—H52D | 0.9800 |
| C16—C17 | 1.4020 (14) | C24—H52E | 0.9800 |
| C17—C18 | 1.4241 (14) | C24—H52F | 0.9800 |
| | | | |
| C1—N1—C23 | 120.30 (8) | C20—C21—C22 | 121.72 (9) |
| C1—N1—C24 | 120.01 (8) | C17—C22—C21 | 121.26 (9) |
| C23—N1—C24 | 119.50 (7) | C1—C2—H2 | 120.00 |
| N1—C1—C2 | 121.37 (8) | C3—C2—H2 | 120.00 |
| N1—C1—C6 | 120.99 (9) | C2—C3—H3 | 119.00 |
| C2—C1—C6 | 117.64 (9) | C4—C3—H3 | 119.00 |
| C1—C2—C3 | 120.61 (9) | C4—C5—H5 | 119.00 |
| C2—C3—C4 | 121.86 (9) | C6—C5—H5 | 119.00 |
| C3—C4—C5 | 117.34 (9) | C1—C6—H6 | 120.00 |
| C3—C4—C7 | 120.70 (8) | C5—C6—H6 | 120.00 |
| C5—C4—C7 | 121.95 (8) | C7—C8—H8 | 119.00 |
| C4—C5—C6 | 121.79 (9) | C9—C8—H8 | 119.00 |
| C1—C6—C5 | 120.70 (9) | C8—C9—H9 | 120.00 |
| C4—C7—C8 | 120.05 (8) | C10—C9—H9 | 120.00 |
| C4—C7—C20 | 121.04 (8) | C10—C11—H11 | 119.00 |
| C8—C7—C20 | 118.88 (9) | C12—C11—H11 | 119.00 |
| C7—C8—C9 | 121.98 (9) | C11—C12—H12 | 120.00 |
| C8—C9—C10 | 120.67 (9) | C13—C12—H12 | 120.00 |
| C9—C10—C11 | 122.31 (9) | C13—C14—H14 | 120.00 |
| C9—C10—C19 | 118.72 (9) | C15—C14—H14 | 120.00 |
| C11—C10—C19 | 118.96 (8) | C14—C15—H15 | 120.00 |
| C10—C11—C12 | 121.59 (9) | C16—C15—H15 | 120.00 |
| C11—C12—C13 | 120.98 (9) | C15—C16—H16 | 120.00 |

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| C12—C13—C14 | 122.18 (9) | C17—C16—H16 | 120.00 |
| C12—C13—C18 | 118.76 (8) | C20—C21—H21 | 119.00 |
| C14—C13—C18 | 119.06 (9) | C22—C21—H21 | 119.00 |
| C13—C14—C15 | 120.62 (9) | C17—C22—H22 | 119.00 |
| C14—C15—C16 | 120.79 (9) | C21—C22—H22 | 119.00 |
| C15—C16—C17 | 120.65 (9) | N1—C23—H52A | 109.00 |
| C16—C17—C18 | 119.11 (9) | N1—C23—H52B | 110.00 |
| C16—C17—C22 | 122.15 (9) | N1—C23—H52C | 109.00 |
| C18—C17—C22 | 118.74 (8) | H52A—C23—H52B | 109.00 |
| C13—C18—C17 | 119.77 (8) | H52A—C23—H52C | 109.00 |
| C13—C18—C19 | 120.24 (8) | H52B—C23—H52C | 109.00 |
| C17—C18—C19 | 119.98 (8) | N1—C24—H52D | 109.00 |
| C10—C19—C18 | 119.46 (8) | N1—C24—H52E | 109.00 |
| C10—C19—C20 | 120.36 (8) | N1—C24—H52F | 109.00 |
| C18—C19—C20 | 120.17 (8) | H52D—C24—H52E | 109.00 |
| C7—C20—C19 | 119.37 (8) | H52D—C24—H52F | 109.00 |
| C7—C20—C21 | 122.44 (9) | H52E—C24—H52F | 109.00 |
| C19—C20—C21 | 118.14 (8) | | |
| | | | |
| C23—N1—C1—C2 | -4.74 (13) | C11—C10—C19—C20 | 179.94 (8) |
| C23—N1—C1—C6 | 175.91 (8) | C10—C11—C12—C13 | 0.52 (14) |
| C24—N1—C1—C2 | -179.66 (8) | C11—C12—C13—C14 | 177.63 (9) |
| C24—N1—C1—C6 | 0.99 (13) | C11—C12—C13—C18 | -1.31 (14) |
| N1—C1—C2—C3 | -177.93 (8) | C12—C13—C14—C15 | -179.17 (9) |
| C6—C1—C2—C3 | 1.44 (13) | C18—C13—C14—C15 | -0.23 (14) |
| N1—C1—C6—C5 | 177.17 (9) | C12—C13—C18—C17 | 179.69 (8) |
| C2—C1—C6—C5 | -2.20 (13) | C12—C13—C18—C19 | 0.73 (13) |
| C1—C2—C3—C4 | 0.79 (14) | C14—C13—C18—C17 | 0.72 (13) |
| C2—C3—C4—C5 | -2.22 (13) | C14—C13—C18—C19 | -178.25 (9) |
| C2—C3—C4—C7 | 176.62 (8) | C13—C14—C15—C16 | -0.61 (15) |
| C3—C4—C5—C6 | 1.44 (13) | C14—C15—C16—C17 | 0.95 (15) |
| C7—C4—C5—C6 | -177.39 (8) | C15—C16—C17—C18 | -0.44 (13) |
| C3—C4—C7—C8 | 62.00 (11) | C15—C16—C17—C22 | 178.41 (9) |
| C3—C4—C7—C20 | -115.98 (10) | C16—C17—C18—C13 | -0.39 (13) |
| C5—C4—C7—C8 | -119.22 (10) | C16—C17—C18—C19 | 178.58 (8) |
| C5—C4—C7—C20 | 62.80 (11) | C22—C17—C18—C13 | -179.28 (8) |
| C4—C5—C6—C1 | 0.77 (14) | C22—C17—C18—C19 | -0.31 (12) |
| C4—C7—C8—C9 | -179.10 (8) | C16—C17—C22—C21 | -178.57 (9) |
| C20—C7—C8—C9 | -1.07 (13) | C18—C17—C22—C21 | 0.30 (13) |
| C4—C7—C20—C19 | 178.40 (8) | C13—C18—C19—C10 | 0.63 (12) |
| C4—C7—C20—C21 | 0.82 (13) | C13—C18—C19—C20 | 179.27 (8) |
| C8—C7—C20—C19 | 0.39 (12) | C17—C18—C19—C10 | -178.34 (8) |
| C8—C7—C20—C21 | -177.19 (8) | C17—C18—C19—C20 | 0.30 (12) |
| C7—C8—C9—C10 | 0.64 (14) | C10—C19—C20—C7 | 0.69 (12) |
| C8—C9—C10—C11 | 179.36 (9) | C10—C19—C20—C21 | 178.38 (8) |
| C8—C9—C10—C19 | 0.47 (13) | C18—C19—C20—C7 | -177.94 (8) |
| C9—C10—C11—C12 | -178.03 (9) | C18—C19—C20—C21 | -0.26 (12) |
| C19—C10—C11—C12 | 0.86 (13) | C7—C20—C21—C22 | 177.84 (9) |
| C9—C10—C19—C18 | 177.52 (8) | C19—C20—C21—C22 | 0.24 (13) |

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|-----------------|------------|-----------------|------------|
| C9—C10—C19—C20 | -1.12 (12) | C20—C21—C22—C17 | -0.26 (14) |
| C11—C10—C19—C18 | -1.41 (12) | | |

Hydrogen-bond geometry (Å, °)

Cg1, Cg2, Cg3, Cg4 and Cg5 are the centroids of the C1–C6, C7–C10/C19/C20, C10–C13/C18/C19, C13–C18 and C17–C22 rings, respectively.

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|---------------------------------------|-------------|---------------|-----------------------|-------------------------|
| C2—H2...Cg2 ⁱ | 0.95 | 2.93 | 3.6043 (15) | 129 |
| C6—H6...Cg5 ⁱⁱ | 0.95 | 2.90 | 3.6495 (15) | 137 |
| C22—H22...Cg1 ⁱⁱⁱ | 0.95 | 2.68 | 3.5499 (15) | 152 |
| C23—H52 <i>A</i> ...Cg3 ⁱ | 0.98 | 2.74 | 3.5994 (15) | 147 |
| C24—H52 <i>E</i> ...Cg4 ⁱⁱ | 0.98 | 2.77 | 3.5284 (15) | 135 |

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