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Crystal structure and Hirshfeld surface analysis of 4-{[(anthracen-9-yl)methyl]amino}benzoic acid dimethylformamide monosolvate

Adeeba Ahmed,[a] Aiman Ahmad,[a] Musheer Ahmad[a] and Valentina A. Kalibabchuk[b]*

[a]Department of Applied Chemistry, ZHCET, Aligarh Muslim University, Aligarh 202002 (UP), India, and [b]Department of General Chemistry, O. O. Bohomolets National Medical University, Shevchenko Blvd. 13, 01601 Kiev, Ukraine. *Correspondence e-mail: kalibabchuk@ukr.net

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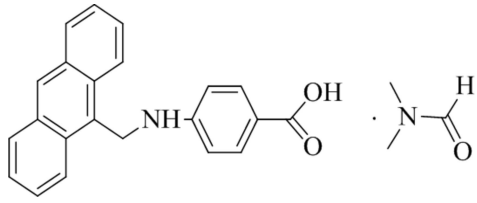
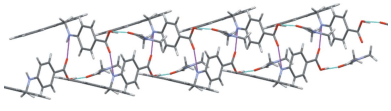
The title compound, $C_{22}H_{17}NO_2{\cdot}C_3H_7NO$, was synthesized by condensation of an aromatic aldehyde with a secondary amine and subsequent reduction. It was crystallized from a dimethylformamide solution as a monosolvate, $C_{22}H_{17}NO_2{\cdot}C_3H_7NO$. The aromatic molecule is non-planar with a dihedral angle between the mean planes of the aniline moiety and the methyl anthracene moiety of 81.36 (8)°. The torsion angle of the $C_{aryl}—CH_2—NH—C_{aryl}$ backbone is 175.9 (2)°. The crystal structure exhibits a three-dimensional supramolecular network, resulting from hydrogen-bonding interactions between the carboxylic OH group and the solvent O atom as well as between the amine functionality and the O atom of the carboxylic group and additional C—H···π interactions. Hirshfeld surface analysis was performed to quantify the intermolecular interactions.

1. Chemical context

Schiff bases belong to a class of organic compounds that are formed by the condensation reaction of a carbonyl carbon with an aliphatic/aromatic amine, resulting in the formation of a characteristic imine bond (–HC═N–). Many Schiff bases exhibit activities of biological and pharmaceutical significance. Moreover, Schiff bases are actively used as organic linkers for building metal complexes with interesting properties.



Here we report the synthesis and crystal structure of a reduced Schiff base that was formed by a condensation reaction of anthraldehyde with 4-amino benzoic acid (PABA). The title compound crystallizes with a dimethylformamide (DMF) solvent molecule in a 1:1: ratio. Both anthraldehyde and PABA have shown anticancer (Pavitha *et al.*, 2017), fluorescence (Obali & Ucan, 2012; Singh *et al.*, 2014), sensing (Zhou *et al.*, 2012), antimicrobial (Vidya, 2016) and magnetic properties (Dianu *et al.*, 2010).



2. Structural commentary

The title molecule is non-planar, with the tricyclic fragment nearly perpendicular to the phenyl ring of the PABA moiety,

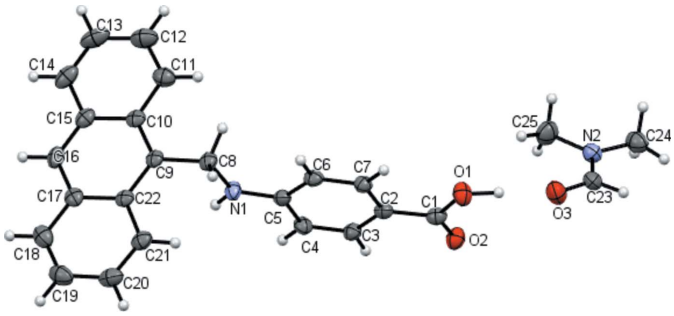


Figure 1
The molecular structures of the components in the title compound. Displacement ellipsoids are drawn at the 50% probability level.

making a dihedral angle of 81.36 (8)° (Fig. 1). The torsion angle of the C_{aryl}—CH_2—NH—C_{aryl} backbone (C9—C8—N1—C5) is 175.9 (2)°. The C8—N1 bond length of 1.452 (3) Å is in agreement with the corresponding bond length of 1.457 (3) Å in the solvent-free compound [CSD (Groom *et al.*, 2016) refcode RUCJIL; Ahmed *et al.*, 2020], just as the bond lengths in the carboxylic group of the title compound, C1—O2 = 1.230 (3), C1—O1 = 1.322 (3) Å, are virtually identical with those of the solvent-free compound [1.238 (3) and 1.325 (3) Å, respectively].

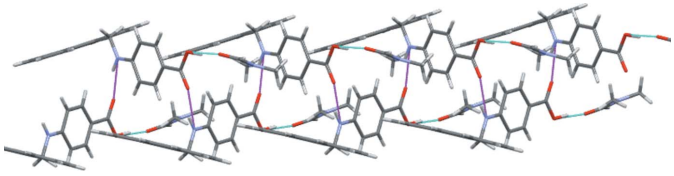


Figure 2
View along [010] showing a layer formed by hydrogen-bonding interactions between the molecule and the solvent. Purple and blue dashed lines represent the N—H···O and O—H···O bonds, respectively.

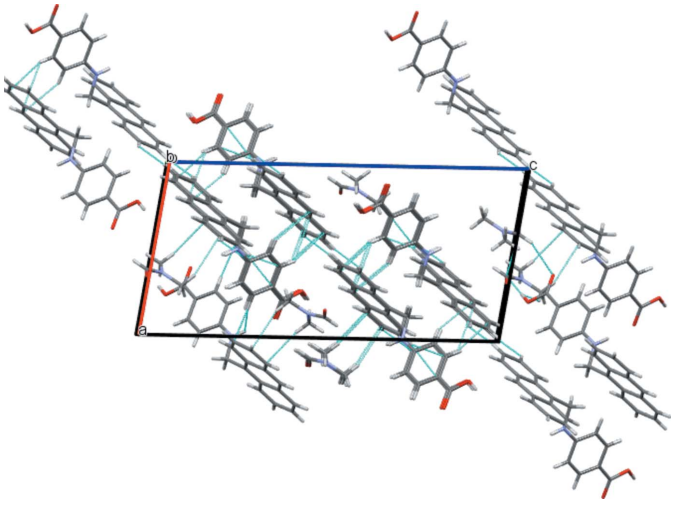


Figure 3
The crystal packing showing C—H···π interactions between the layers, building up a three-dimensional network.

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*5 and *Cg*7 are the centroids of the 10-membered ring system C9–C22 and of the 14-membered anthracene moiety, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3	1.02 (4)	1.59 (4)	2.590 (3)	167 (4)
N1—H1A···O2^{i}	0.88 (1)	2.13 (1)	2.973 (3)	160 (1)
C18—H18···O3^{ii}	0.95 (1)	2.40 (1)	3.277 (4)	154 (1)
C6—H6···*Cg*7^{iii}	0.95	2.80 (1)	3.552 (2)	137 (1)
C7—H7···*Cg*5^{iii}	0.95	2.99 (1)	3.646 (3)	138 (1)

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

3. Supramolecular features

Classical hydrogen-bonding interactions between the carboxylic OH group (O1) and the solvent O atom (O3) as well as between the amine functionality (N1) and the O atom of the carboxylic group (O2) lead to the formation of supramolecular layers extending parallel to (10$\bar{1}$) (Fig. 2, Table 1). C—H···π interactions involving the phenyl C—H groups of PABA as donor groups and the π system of the anthracene moiety link adjacent layers into a three-dimensional network (Fig. 3, Table 1).

4. Hirshfeld Surface Analysis

Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *CrystalExplorer* (Turner *et al.*, 2017). The Hirshfeld surfaces are colour-mapped with the normalized contact distance, d_{norm}, varying from red (distances shorter than the sum of the van der Waals radii) through white to blue (distances longer than the sum of the van der Waals radii). The positions of the O—H···O and N—H···O hydrogen bonds between the molecules are indicated by the red regions on the Hirshfeld surface (Fig. 4).

The two-dimensional fingerprint plot (Fig. 5*a*) and those delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) N···H/H···N and (*e*) O···H/H···O interactions reveal contributions of

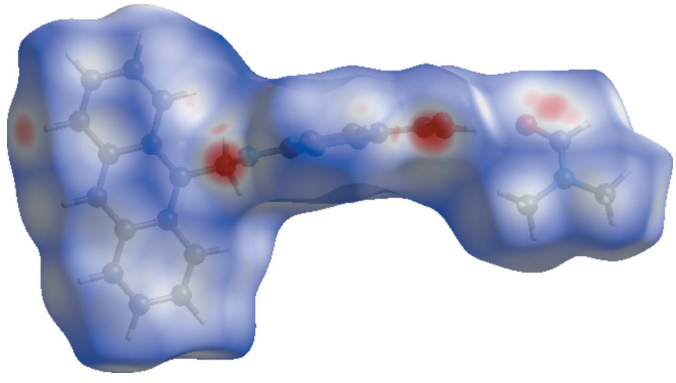


Figure 4
Hirshfeld surface of the two molecules in the title compound mapped over d_{norm}, in the colour range −0. 461 to 1.471 a.u..

47.9%, 34.2%, 0.6% and 13.7%, respectively, to the overall surface.

5. Database survey

Next to the solvent-free crystal structure (RUCJIL; Ahmed *et al.*, 2020), a search of the Cambridge Structural Database (CSD,Version 5.40, update August 2019; Groom *et al.*, 2016) for the *N*-(anthracen-9-ylmethyl)aniline skeleton gave six hits, five polymeric metal complexes of the ligand 5-[(anthracen-9-ylmethyl)amino]isophthalic acid containing gadolinium (VOLSOG, VOLSUM, VOLTAT, VOLTIB; Singh *et al.*, 2014) and cadmium (EYUMOC; Yan *et al.*, 2016) as well as an organic molecule with a calix(4)arene ring (Bu *et al.*, 2004). In these structures, the bridging C—N bond length varies from ≃ 1.389 to 1.494 Å, compared to the C8—N1 bond length of 1.452 (3) Å in the title structure.

6. Synthesis and crystallization

The Schiff base was synthesized and subsequently reduced by a reported procedure (Ahmed *et al.*, 2020). To this reduced ligand (0.15 mmol), ethanol and dimethylformamide were added in an equal volume ratio, and the mixture was heated under reflux for 3–4 h at 353 K. The solution was then allowed to cool to room temperature, filtered and kept for slow evaporation. After 10 to 12 d, small colourless block-like crystals began to grow that were dried and characterized by single crystal X-ray diffraction.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms bound to N or O atoms were located in a difference-Fourier map and were freely refined, while the C-bound hydrogen atoms were included in calculated positions and allowed to ride on their parent C atom: C—H = 0.93–0.97 Å with U_{iso}(H) = 1.2U_{eq}(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}NO_2{\cdot}C_3H_7NO$
M_r	400.48
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	10.6878 (9), 8.9088 (7), 21.9503 (19)
β (°)	99.049 (3)
V (Å^3)	2064.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.36 × 0.28 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.368, 0.746
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	31593, 3668, 2477
R_{int}	0.139
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.184, 1.12
No. of reflections	3668
No. of parameters	278
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.37

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *olex2.solve* (Bourhis *et al.*, 2015), *olex2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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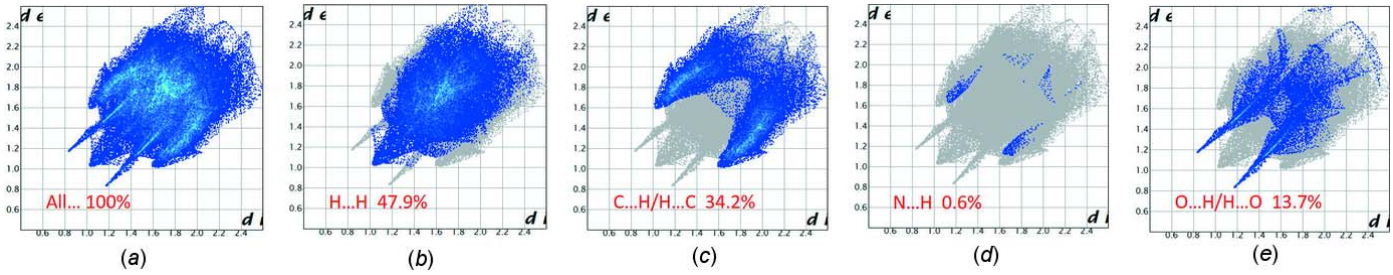

Figure 5
(*a*) Two-dimensional fingerprint plot of the title compound, and those delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) N···H/H···N and (*e*) O···H/H···O interactions.

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Acta Cryst. (2020). E**76**, 728-731 [https://doi.org/10.1107/S2056989020005393]

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Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *olex2.solve* (Bourhis *et al.*, 2015); program(s) used to refine structure: *olex2.refine* (Bourhis *et al.*, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

4-{[(Anthracen-9-yl)methyl]amino}benzoic acid dimethylformamide monosolvate#

Crystal data

$C_{22}H_{17}NO_2 \cdot C_3H_7NO$
$M_r = 400.48$
Monoclinic, $P2_1/n$
$a = 10.6878$ (9) Å
$b = 8.9088$ (7) Å
$c = 21.9503$ (19) Å
$\beta = 99.049$ (3)°
$V = 2064.0$ (3) Å^3
$Z = 4$
$F(000) = 848.4030$
$D_x = 1.289$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4326 reflections
$\theta = 3.2–28.1°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Block, colourless
0.36 × 0.28 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
$T_{min} = 0.368$, $T_{max} = 0.746$
31593 measured reflections
3668 independent reflections
2477 reflections with $I \geq 2u(I)$
$R_{int} = 0.139$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.0°$
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.184$
$S = 1.12$
3668 reflections
278 parameters
0 restraints
41 constraints
Primary atom site location: iterative
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0846P)^2 + 0.3653P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.73134 (18)	0.7445 (2)	0.43603 (9)	0.0355 (5)
O2	0.88916 (17)	0.7377 (2)	0.38033 (9)	0.0323 (5)
O3	0.83886 (19)	0.9615 (2)	0.50335 (9)	0.0400 (5)
N1	0.49557 (19)	0.2754 (2)	0.23347 (11)	0.0271 (5)
H1a	0.52980 (19)	0.2410 (2)	0.20230 (11)	0.0326 (7)*
N2	0.8603 (2)	1.1906 (2)	0.46049 (11)	0.0319 (6)
C1	0.7855 (2)	0.6922 (3)	0.39023 (13)	0.0271 (6)
C2	0.7105 (2)	0.5787 (3)	0.35193 (12)	0.0239 (6)
C3	0.7566 (2)	0.5171 (3)	0.30121 (12)	0.0262 (6)
H3	0.8380 (2)	0.5456 (3)	0.29315 (12)	0.0314 (7)*
C4	0.6864 (2)	0.4164 (3)	0.26299 (13)	0.0270 (6)
H4	0.7197 (2)	0.3763 (3)	0.22878 (13)	0.0324 (8)*
C5	0.5653 (2)	0.3715 (3)	0.27377 (12)	0.0242 (6)
C6	0.5206 (2)	0.4299 (3)	0.32576 (12)	0.0263 (6)
H6	0.4407 (2)	0.3988 (3)	0.33498 (12)	0.0316 (7)*
C7	0.5920 (2)	0.5320 (3)	0.36341 (12)	0.0251 (6)
H7	0.5597 (2)	0.5715 (3)	0.39801 (12)	0.0302 (7)*
C8	0.3682 (2)	0.2265 (3)	0.23901 (13)	0.0272 (6)
H8a	0.3697 (2)	0.1682 (3)	0.27751 (13)	0.0327 (8)*
H8b	0.3128 (2)	0.3149 (3)	0.24074 (13)	0.0327 (8)*
C9	0.3172 (2)	0.1300 (3)	0.18389 (12)	0.0234 (6)
C10	0.2375 (2)	0.1918 (3)	0.13285 (12)	0.0248 (6)
C11	0.1944 (3)	0.3436 (3)	0.13080 (14)	0.0344 (7)
H11	0.2224 (3)	0.4081 (3)	0.16466 (14)	0.0412 (9)*
C12	0.1145 (3)	0.3979 (4)	0.08172 (16)	0.0452 (8)
H12	0.0856 (3)	0.4987 (4)	0.08225 (16)	0.0543 (10)*
C13	0.0737 (3)	0.3074 (4)	0.03015 (16)	0.0456 (9)
H13	0.0174 (3)	0.3471 (4)	−0.00384 (16)	0.0548 (10)*
C14	0.1141 (3)	0.1640 (4)	0.02867 (14)	0.0372 (7)
H14	0.0880 (3)	0.1048 (4)	−0.00706 (14)	0.0447 (9)*
C15	0.1955 (2)	0.0998 (3)	0.07979 (12)	0.0282 (6)
C16	0.2339 (2)	−0.0494 (3)	0.07998 (13)	0.0289 (7)
H16	0.2064 (2)	−0.1097 (3)	0.04472 (13)	0.0347 (8)*
C17	0.3112 (2)	−0.1129 (3)	0.13030 (12)	0.0266 (6)
C18	0.3469 (3)	−0.2670 (3)	0.13064 (15)	0.0350 (7)
H18	0.3170 (3)	−0.3283 (3)	0.09599 (15)	0.0420 (9)*
C19	0.4230 (3)	−0.3272 (3)	0.17973 (16)	0.0407 (8)
H19	0.4447 (3)	−0.4306 (3)	0.17957 (16)	0.0489 (10)*
C20	0.4701 (3)	−0.2375 (3)	0.23099 (15)	0.0368 (7)
H20	0.5252 (3)	−0.2804 (3)	0.26469 (15)	0.0441 (9)*
C21	0.4378 (2)	−0.0896 (3)	0.23285 (13)	0.0306 (7)
H21	0.4707 (2)	−0.0312 (3)	0.26793 (13)	0.0367 (8)*
C22	0.3555 (2)	−0.0209 (3)	0.18322 (12)	0.0235 (6)
C23	0.8782 (3)	1.0922 (3)	0.50634 (14)	0.0318 (7)
H23	0.9249 (3)	1.1247 (3)	0.54448 (14)	0.0381 (8)*

C24	0.9129 (3)	1.3401 (3)	0.46883 (15)	0.0401 (8)
H24a	0.8440 (3)	1.4139 (3)	0.4638 (9)	0.0602 (12)*
H24b	0.9620 (16)	1.3491 (7)	0.5103 (3)	0.0602 (12)*
H24c	0.9684 (15)	1.3586 (9)	0.4381 (6)	0.0602 (12)*
C25	0.7882 (3)	1.1510 (4)	0.40096 (14)	0.0445 (8)
H25a	0.8462 (3)	1.136 (2)	0.3711 (3)	0.0668 (12)*
H25b	0.7411 (15)	1.0580 (13)	0.4049 (2)	0.0668 (12)*
H25c	0.7286 (14)	1.2320 (11)	0.3868 (5)	0.0668 (12)*
H1	0.776 (4)	0.836 (4)	0.4571 (18)	0.085 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0360 (12)	0.0387 (12)	0.0343 (12)	−0.0078 (9)	0.0132 (9)	−0.0087 (10)
O2	0.0293 (11)	0.0377 (11)	0.0307 (11)	−0.0076 (8)	0.0071 (9)	−0.0032 (9)
O3	0.0511 (13)	0.0329 (12)	0.0356 (13)	−0.0006 (9)	0.0058 (10)	−0.0041 (10)
N1	0.0206 (11)	0.0305 (12)	0.0311 (13)	−0.0044 (9)	0.0066 (10)	−0.0092 (10)
N2	0.0321 (13)	0.0264 (12)	0.0366 (15)	0.0015 (10)	0.0039 (11)	−0.0002 (11)
C1	0.0242 (15)	0.0293 (15)	0.0288 (16)	0.0008 (11)	0.0071 (12)	0.0040 (12)
C2	0.0220 (13)	0.0238 (13)	0.0260 (15)	0.0027 (10)	0.0043 (11)	0.0031 (11)
C3	0.0201 (13)	0.0254 (14)	0.0331 (16)	−0.0019 (10)	0.0045 (11)	0.0012 (12)
C4	0.0240 (14)	0.0272 (14)	0.0311 (16)	0.0007 (11)	0.0088 (11)	−0.0040 (12)
C5	0.0215 (13)	0.0230 (13)	0.0278 (15)	0.0016 (10)	0.0030 (11)	0.0018 (12)
C6	0.0199 (13)	0.0284 (14)	0.0316 (16)	0.0005 (11)	0.0070 (11)	0.0012 (12)
C7	0.0230 (14)	0.0275 (14)	0.0255 (15)	0.0017 (11)	0.0055 (11)	−0.0011 (12)
C8	0.0197 (14)	0.0317 (15)	0.0309 (16)	−0.0039 (11)	0.0060 (11)	−0.0039 (12)
C9	0.0166 (13)	0.0278 (14)	0.0267 (15)	−0.0037 (10)	0.0064 (11)	−0.0007 (12)
C10	0.0179 (13)	0.0265 (14)	0.0311 (16)	−0.0033 (10)	0.0075 (11)	0.0036 (12)
C11	0.0327 (16)	0.0330 (16)	0.0387 (18)	0.0027 (12)	0.0097 (13)	0.0042 (14)
C12	0.0374 (18)	0.0412 (18)	0.057 (2)	0.0063 (14)	0.0066 (16)	0.0160 (17)
C13	0.0301 (17)	0.058 (2)	0.047 (2)	0.0023 (15)	−0.0001 (15)	0.0250 (17)
C14	0.0266 (15)	0.0536 (19)	0.0307 (17)	−0.0107 (14)	0.0021 (13)	0.0099 (15)
C15	0.0212 (14)	0.0355 (15)	0.0284 (16)	−0.0060 (11)	0.0055 (11)	0.0037 (13)
C16	0.0240 (14)	0.0356 (16)	0.0281 (16)	−0.0089 (11)	0.0066 (12)	−0.0044 (13)
C17	0.0209 (13)	0.0284 (14)	0.0326 (16)	−0.0046 (11)	0.0106 (12)	−0.0013 (12)
C18	0.0336 (16)	0.0291 (15)	0.045 (2)	−0.0057 (12)	0.0159 (14)	−0.0033 (14)
C19	0.0361 (17)	0.0262 (15)	0.062 (2)	0.0008 (13)	0.0139 (16)	0.0051 (15)
C20	0.0260 (15)	0.0352 (16)	0.048 (2)	0.0010 (12)	0.0036 (14)	0.0132 (15)
C21	0.0217 (14)	0.0340 (15)	0.0358 (17)	−0.0047 (11)	0.0040 (12)	0.0039 (13)
C22	0.0168 (13)	0.0256 (13)	0.0290 (15)	−0.0029 (10)	0.0065 (11)	0.0027 (12)
C23	0.0307 (15)	0.0281 (15)	0.0360 (18)	0.0041 (12)	0.0036 (13)	−0.0066 (13)
C24	0.0380 (18)	0.0304 (16)	0.053 (2)	−0.0011 (13)	0.0099 (15)	0.0012 (15)
C25	0.047 (2)	0.049 (2)	0.0341 (18)	−0.0011 (15)	−0.0030 (15)	0.0005 (15)

Geometric parameters (Å, º)

O1—C1	1.322 (3)	C11—H11	0.9500
O1—H1	1.02 (4)	C11—C12	1.354 (4)

O2—C1	1.230 (3)	C12—H12	0.9500
O3—C23	1.236 (3)	C12—C13	1.402 (5)
N1—H1a	0.8800	C13—H13	0.9500
N1—C5	1.365 (3)	C13—C14	1.351 (4)
N1—C8	1.452 (3)	C14—H14	0.9500
N2—C23	1.326 (4)	C14—C15	1.427 (4)
N2—C24	1.446 (3)	C15—C16	1.391 (4)
N2—C25	1.452 (4)	C16—H16	0.9500
C1—C2	1.470 (4)	C16—C17	1.392 (4)
C2—C3	1.399 (4)	C17—C18	1.424 (4)
C2—C7	1.393 (3)	C17—C22	1.439 (4)
C3—H3	0.9500	C18—H18	0.9500
C3—C4	1.368 (4)	C18—C19	1.355 (4)
C4—H4	0.9500	C19—H19	0.9500
C4—C5	1.410 (3)	C19—C20	1.407 (4)
C5—C6	1.405 (4)	C20—H20	0.9500
C6—H6	0.9500	C20—C21	1.365 (4)
C6—C7	1.376 (4)	C21—H21	0.9500
C7—H7	0.9500	C21—C22	1.426 (4)
C8—H8a	0.9900	C23—H23	0.9500
C8—H8b	0.9900	C24—H24a	0.9800
C8—C9	1.514 (4)	C24—H24b	0.9800
C9—C10	1.408 (4)	C24—H24c	0.9800
C9—C22	1.406 (3)	C25—H25a	0.9800
C10—C11	1.427 (4)	C25—H25b	0.9800
C10—C15	1.437 (4)	C25—H25c	0.9800

H1—O1—C1	114 (2)	H13—C13—C12	119.91 (18)
C5—N1—H1a	118.07 (14)	C14—C13—C12	120.2 (3)
C8—N1—H1a	118.07 (14)	C14—C13—H13	119.91 (19)
C8—N1—C5	123.9 (2)	H14—C14—C13	119.40 (19)
C24—N2—C23	120.4 (2)	C15—C14—C13	121.2 (3)
C25—N2—C23	121.1 (2)	C15—C14—H14	119.40 (18)
C25—N2—C24	118.6 (2)	C14—C15—C10	118.9 (3)
O2—C1—O1	122.2 (3)	C16—C15—C10	119.2 (2)
C2—C1—O1	114.4 (2)	C16—C15—C14	121.9 (3)
C2—C1—O2	123.4 (2)	H16—C16—C15	119.03 (16)
C3—C2—C1	119.8 (2)	C17—C16—C15	121.9 (2)
C7—C2—C1	122.1 (2)	C17—C16—H16	119.03 (16)
C7—C2—C3	118.1 (2)	C18—C17—C16	121.4 (3)
H3—C3—C2	119.41 (15)	C22—C17—C16	119.2 (2)
C4—C3—C2	121.2 (2)	C22—C17—C18	119.4 (2)
C4—C3—H3	119.41 (16)	H18—C18—C17	119.59 (17)
H4—C4—C3	119.59 (16)	C19—C18—C17	120.8 (3)
C5—C4—C3	120.8 (2)	C19—C18—H18	119.59 (17)
C5—C4—H4	119.59 (15)	H19—C19—C18	119.81 (17)
C4—C5—N1	119.4 (2)	C20—C19—C18	120.4 (3)
C6—C5—N1	122.6 (2)	C20—C19—H19	119.81 (17)

C6—C5—C4	118.0 (2)	H20—C20—C19	119.60 (17)
H6—C6—C5	119.79 (15)	C21—C20—C19	120.8 (3)
C7—C6—C5	120.4 (2)	C21—C20—H20	119.60 (18)
C7—C6—H6	119.79 (15)	H21—C21—C20	119.32 (18)
C6—C7—C2	121.5 (2)	C22—C21—C20	121.4 (3)
H7—C7—C2	119.26 (15)	C22—C21—H21	119.32 (16)
H7—C7—C6	119.26 (15)	C17—C22—C9	119.6 (2)
H8a—C8—N1	109.85 (14)	C21—C22—C9	123.2 (2)
H8b—C8—N1	109.85 (14)	C21—C22—C17	117.2 (2)
H8b—C8—H8a	108.3	N2—C23—O3	125.1 (3)
C9—C8—N1	109.2 (2)	H23—C23—O3	117.46 (17)
C9—C8—H8a	109.85 (14)	H23—C23—N2	117.46 (16)
C9—C8—H8b	109.85 (14)	H24a—C24—N2	109.5
C10—C9—C8	120.7 (2)	H24b—C24—N2	109.5
C22—C9—C8	118.8 (2)	H24b—C24—H24a	109.5
C22—C9—C10	120.4 (2)	H24c—C24—N2	109.5
C11—C10—C9	123.2 (2)	H24c—C24—H24a	109.5
C15—C10—C9	119.7 (2)	H24c—C24—H24b	109.5
C15—C10—C11	117.2 (2)	H25a—C25—N2	109.5
H11—C11—C10	119.22 (16)	H25b—C25—N2	109.5
C12—C11—C10	121.6 (3)	H25b—C25—H25a	109.5
C12—C11—H11	119.22 (19)	H25c—C25—N2	109.5
H12—C12—C11	119.52 (19)	H25c—C25—H25a	109.5
C13—C12—C11	121.0 (3)	H25c—C25—H25b	109.5
C13—C12—H12	119.52 (18)		

Hydrogen-bond geometry (Å, º)

*Cg*5 and *Cg*7 are the centroids of the 10-membered ring system C9–C22 and of the 14-membered anthracene moiety, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3	1.02 (4)	1.59 (4)	2.590 (3)	167 (4)
N1—H1A···O2^{i}	0.88 (1)	2.13 (1)	2.973 (3)	160 (1)
C18—H18···O3^{ii}	0.95 (1)	2.40 (1)	3.277 (4)	154 (1)
C6—H6···*Cg*7^{iii}	0.95	2.80 (1)	3.552 (2)	137 (1)
C7—H7···*Cg*5^{iii}	0.95	2.99 (1)	3.646 (3)	138 (1)

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2.