Niels Thorup,[a]*
Jørgen Eskildsen[b]‡ and
Jørn B. Christensen[b]

[a]Department of Chemistry, Technical University of Denmark, Kemitorvet, DTU-207, DK-2800 Kgs. Lyngby, Denmark, and [b]Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

‡ Present address: Acadia Pharmaceuticals AB PA, Hanssonsväg 35, S-20512 Malmö, Sweden.

Correspondence e-mail: nt@kemi.dtu.dk

Key indicators

Single-crystal X-ray study
$T = 120$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.099
Data-to-parameter ratio = 11.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Acenaphtho[1,2-*b*]pyrazine

In the crystal structure of acenaphtho[1,2-*b*]pyrazine (or 7,10-diazafluoranthene), $C_{14}H_8N_2$, the molecule has crystallographic *m* symmetry, but the observed symmetry is very close to *mm*2. The structure contains dimers of face-to-face antiparallel molecules.

Comment

Fluoranthene forms a series of 2:1 radical cation salts with anions such as PF_6^- and AsF_6^- (Enkelmann *et al.*, 1982). 10*c*-Azoniafluoranthene forms a 1:1 radical cation salt with the anion PF_6^- (Boubekeur *et al.*, 1989). The present molecule, 7,10-diazafluoranthene or acenaphtho[1,2-*b*]pyrazine, (I), is of interest as a modified fluoranthene with nitrogen substitution along the periphery.

(I)
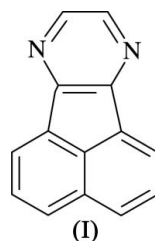
The molecule has crystallographic *m* symmetry. As expected, the observed symmetry is very close to *mm*2 (C_{2v}). The structure contains dimers of face-to-face antiparallel
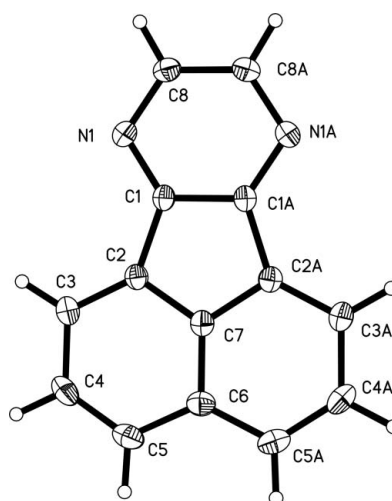
Figure 1
The molecular structure of acenaphtho[1,2-*b*]pyrazine with the atomic numbering scheme. The symbol A refers to symmetry code (i) in Table 1. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.
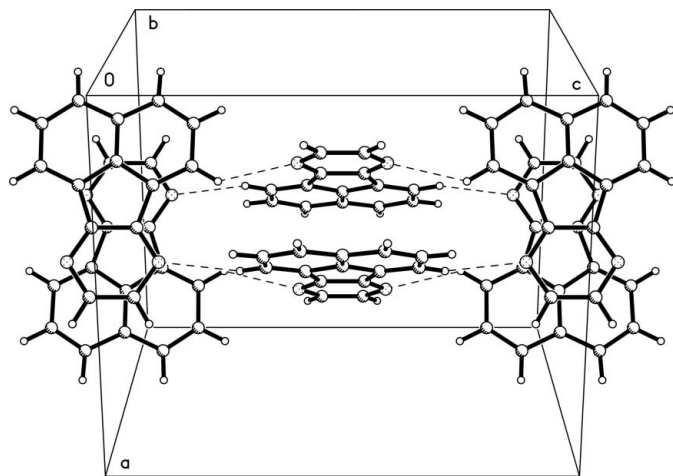
Figure 2
Packing viewed approximately along the *b*-axis direction. Dashed lines represent the weak C—H···N hydrogen bond detailed in Table 2.

molecules. The interplanar distance within a dimer is 3.417 (2) Å. The dimers probably interact *via* a weak C—H···N hydrogen bond (see Table 2). The interacting dimers are stacked orthogonally to each other (see Fig. 2). The intermolecular attractions appear to be rather weak, which is in good accordance with the observed low melting point (*ca* 419 K).

Experimental

Acenaphtho[1,2-*b*]pyrazine was prepared as previously reported by Eskildsen & Christensen (2004). Crystals for X-ray analysis were obtained by slow evaporation of a solution in ethanol of a sublimed sample.

Crystal data

$C_{14}H_8N_2$	Mo $K\alpha$ radiation
$M_r = 204.22$	Cell parameters from 7188
Tetragonal, $P4_2/mbc$	reflections
$a = 11.9243\ (2)$ Å	$\theta = 2.4$–$26.4°$
$c = 14.4040\ (3)$ Å	$\mu = 0.08$ mm^{-1}
$V = 2048.09\ (6)$ Å^3	$T = 120\ (2)$ K
$Z = 8$	Prism, yellow
$D_x = 1.325$ Mg m^{-3}	$0.30 \times 0.09 \times 0.06$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	1088 independent reflections
	910 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.052$
Absorption correction: multi-scan	$\theta_{max} = 26.4°$
(*SADABS*; Sheldrick, 2003)	$h = -14 \rightarrow 14$
$T_{min} = 0.900$, $T_{max} = 0.995$	$k = -14 \rightarrow 14$
17778 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$+ 0.8729P]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} < 0.001$
1088 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
93 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
All H-atom parameters refined	Extinction correction: *SHELXTL*
	Extinction coefficient: 0.0035 (6)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3347 (17)	C3—C4	1.424 (2)
N1—C8	1.3489 (18)	C4—C5	1.382 (2)
C1—C1^i	1.428 (3)	C5—C6	1.4251 (18)
C1—C2	1.4734 (19)	C6—C7	1.406 (3)
C2—C3	1.376 (2)	C8—C8^i	1.392 (3)
C2—C7	1.4179 (17)		
C1—N1—C8	113.94 (12)	C5—C4—C3	122.91 (14)
N1—C1—C1^i	122.76 (8)	C4—C5—C6	120.27 (15)
N1—C1—C2	128.87 (12)	C7—C6—C5	115.83 (10)
C1^i—C1—C2	108.36 (8)	C5—C6—C5^i	128.3 (2)
C3—C2—C7	119.34 (13)	C6—C7—C2	123.81 (9)
C3—C2—C1	135.20 (13)	C2^i—C7—C2	112.38 (17)
C7—C2—C1	105.45 (12)	N1—C8—C8^i	123.29 (8)
C2—C3—C4	117.84 (14)		

Symmetry code: (i) $x, y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{ii}	0.982 (17)	2.605 (16)	3.3663 (19)	134.5 (12)

Symmetry code: (ii) $-y, x, -z + \frac{1}{2}$.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* (Sheldrick, 2001) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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