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6-*n*-Butylacenaphtho[1,2-*b*]benzo[*h*]-quinoline

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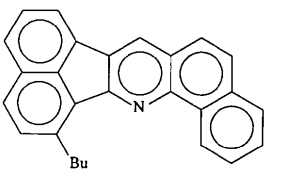
Abstract

The molecule of the title compound, $C_{27}H_{21}N$, is planar except for the extended *n*-butyl chain which is perpendicular to the molecular plane. The crystal structure is stabilized by van der Waals interactions.

Comment

Butylation of polycyclic azaarenes (PAA) improves their solubility in common organic solvents and thus enhances their potential as substrates for molecular recognition. They are relatively rigid planar hosts for metal ions and organic molecules (Bell & Firestone, 1986). In an attempt to synthesize monoalkylated PAA with a butyl group exclusively in the semi-bay region of the acenaphthylene moiety, which is highly influenced by the position of the heteroatoms, we have developed a new route involving simple alkyllithiums (Ray, Roy & Kar, 1996). As part of studies on the synthesis, characterization and bioactivity of polycyclic aromatic hydrocarbon derivatives, the structure of the title compound, (I), has been determined.



(I)

An ellipsoid plot of (I) with the atom-numbering scheme is shown in Fig. 1. The bond lengths and angles observed in this structure are normal. The aromatic ring system is planar with a dihedral angle of only 1.78 (3)° between the planes of the benzoquinoline and naphthalene moieties. The butyl group is perpendicular to the plane of the rest of the molecule. The N atom is involved in short intramolecular contacts with C3 [2.818 (2) Å] and C24 [3.225 (2) Å]. The crystal structure is stabilized by van der Waals interactions.

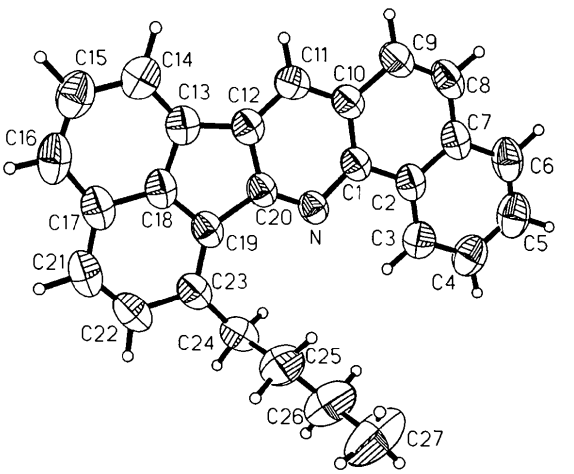


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Single crystals of the title compound were obtained by slow evaporation from a chloroform–tetrachloromethane mixture.

Crystal data

$C_{27}H_{21}N$
M_r = 359.45
Monoclinic
$P2_1/c$
a = 19.289 (4) Å
b = 6.0580 (10) Å
c = 16.792 (3) Å
β = 98.230 (10)°
V = 1942.0 (6) Å^3
Z = 4
D_x = 1.229 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 43 reflections
θ = 5.3–12.6°
μ = 0.071 mm^{-1}
T = 293 (2) K
Rectangular slab cut from bigger crystal
0.98 × 0.54 × 0.36 mm
Yellow

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Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
5788 measured reflections
4448 independent reflections
2609 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.50°$
$h = -25 \rightarrow 24$
$k = -7 \rightarrow 1$
$l = -1 \rightarrow 21$
3 standard reflections
every 97 reflections
intensity decay: <3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.138$
$S = 0.891$
4448 reflections
337 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.214$ e Å^{-3}
$\Delta\rho_{min} = -0.163$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

N—C20	1.315 (2)	C13—C14	1.370 (2)
N—C1	1.360 (2)	C13—C18	1.413 (2)
C1—C10	1.412 (2)	C14—C15	1.406 (3)
C1—C2	1.445 (2)	C15—C16	1.365 (3)
C2—C3	1.401 (2)	C16—C17	1.411 (3)
C2—C7	1.410 (2)	C17—C18	1.398 (2)
C3—C4	1.373 (2)	C17—C21	1.409 (2)
C4—C5	1.389 (3)	C18—C19	1.406 (2)
C5—C6	1.350 (3)	C19—C23	1.376 (2)
C6—C7	1.406 (2)	C19—C20	1.476 (2)
C7—C8	1.421 (2)	C21—C22	1.369 (3)
C8—C9	1.344 (2)	C22—C23	1.429 (2)
C9—C10	1.437 (2)	C23—C24	1.489 (2)
C10—C11	1.406 (2)	C24—C25	1.528 (3)
C11—C12	1.360 (2)	C25—C26	1.484 (3)
C12—C20	1.435 (2)	C26—C27	1.511 (4)
C12—C13	1.468 (2)		
C20—N—C1	116.45 (12)	C17—C18—C13	122.93 (15)
N—C1—C10	122.74 (13)	C19—C18—C13	112.50 (13)
N—C1—C2	117.63 (13)	C23—C19—C20	134.31 (14)
C11—C12—C13	133.84 (14)	C18—C19—C20	105.71 (12)
C20—C12—C13	108.03 (12)	N—C20—C12	124.98 (12)
C14—C13—C18	118.89 (15)	N—C20—C19	127.10 (12)
C14—C13—C12	135.27 (15)	C12—C20—C19	107.92 (12)
C18—C13—C12	105.83 (13)	C19—C23—C22	115.8 (2)
C18—C17—C21	115.0 (2)	C19—C23—C24	123.23 (14)
C18—C17—C16	116.5 (2)	C23—C24—C25	112.15 (15)
C21—C17—C16	128.5 (2)	C26—C25—C24	114.3 (2)
C17—C18—C19	124.57 (15)	C25—C26—C27	113.5 (3)
C19—C23—C24—C25	84.7 (2)	C23—C24—C25—C26	−175.1 (2)
C22—C23—C24—C25	−93.9 (2)	C24—C25—C26—C27	−179.4 (3)

The structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from difference Fourier maps and refined isotropically. Program used for geometrical calculations: *PARST* (Nardelli, 1983).

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: MU1329). Services for accessing these data are described at the back of the journal.

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N-(4-Nitrophenyl)-*trans*-2-aminocyclohexanol

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Abstract

The phenyl ring in $C_{12}H_{16}N_2O_3$ is planar and the nitro group is distorted from coplanarity with it. The cyclohexane ring adopts a boat conformation. The molecules exist as centrosymmetrically-related dimers and pack as linear chains parallel to the *b* axis.

Comment

The β-aminoalcohol sequence plays an important part in organic and in medicinal chemistry (Goodman & Gilman, 1980). Specifically, the β-aminoalcohol subunit has been of particular value in the study of acetylcholine metabolism in intact nerve-terminal preparations (Rogers *et al.*, 1989). The crystal structure determination

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