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9-Benzylacridine

Artur Sikorski, Katarzyna Kowalska, Karol Krzymiński and Jerzy Błażejowski*

University of Gdańsk, Faculty of Chemistry, J. Sobieskiego 18, 80-952 Gdańsk, Poland

Correspondence e-mail: bla@chem.univ.gda.pl

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Key indicators

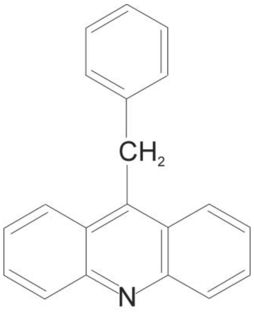
Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.110
Data-to-parameter ratio = 13.2

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

In the crystal structure of the title compound, $C_{20}H_{15}N$, molecules related by a centre of symmetry are arranged in pairs that are stabilized *via* π–π interactions between the acridine units. Adjacent pairs, with the acridine ring systems arranged in a herringbone pattern, are linked through a network of C—H$\cdots\pi$ interactions. Non-specific dispersive interactions between layers formed from pairs in the *ab* plane stabilize the crystal structure. The acridine ring systems in pairs are parallel, while in adjacent pairs they are inclined to each other at 78.3 (2)°. The acridine systems and phenyl ring are oriented at 73.3 (2)° to each other.

Comment

Interest in compounds exhibiting chemiluminogenic ability has a long history (Gundermann & McCapra, 1987; Dodeigne *et al.*, 2000; Zomer & Jacquemijns, 2001). In this context, acridinium derivatives containing a substituent at C9 facilitating the oxidation of the molecules and their transformation to light-emitting 9-acridinones appear to be very promising (Gundermann & McCapra, 1987; Rak *et al.*, 1999; Dodeigne *et al.*, 2000; Zomer & Jacquemijns, 2001). Such compounds can serve as analytical indicators of substances affecting the efficiency of chemiluminescence or as fragments of chemiluminescent labels used in medicinal, environmental and chemical assays of macromolecules (Dodeigne *et al.*, 2000; Zomer & Jacquemijns, 2001). We have been investigating the chemiluminogenic ability of 10-methyl-9-phenoxycarbonylacridinium (Rak *et al.*, 1999) and 10-methyl-9-cyanoacridinium (Wróblewska, Huta, Midyanyj *et al.*, 2004) cations and the possible uses of the latter entity in the assay of nucleophiles (Wróblewska, Huta, Patsay *et al.*, 2004).



(I)

A disadvantage of the above-mentioned acridinium derivatives is the relatively low efficiency of their chemiluminescence. This encouraged us to search for new acridinium-based derivatives able to react efficiently with oxidizing agents to

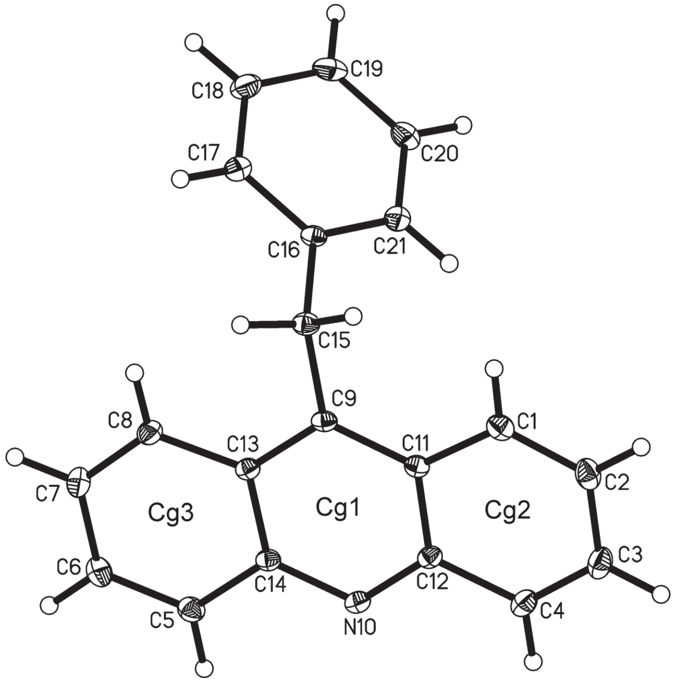


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 25% probability level and H atoms are shown as small spheres of arbitrary radius.

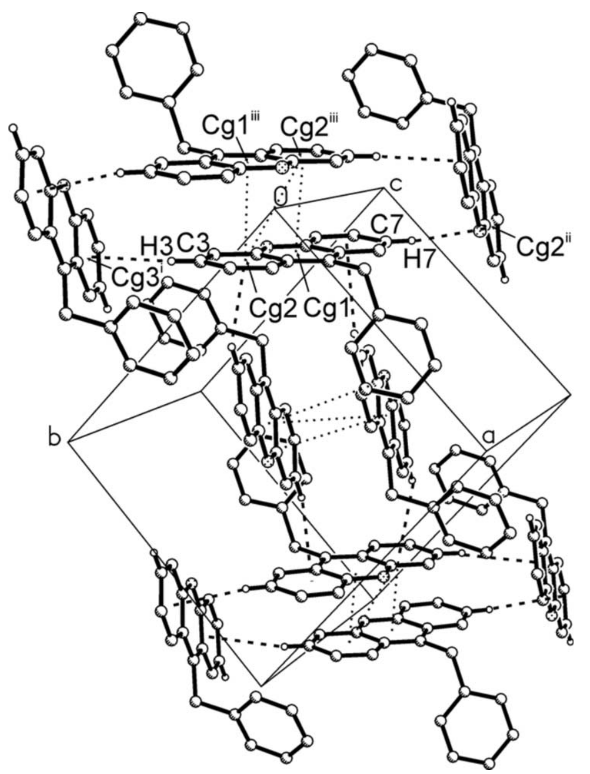


Figure 2
The arrangement of the molecules of (I) in the crystal structure. The C—H$\cdots\pi$ interactions are represented by dashed lines and π–π interactions by dotted lines. H atoms not involved in these interactions have been omitted. [Symmetry codes: (i) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $-x, -y, -z$.]

produce light. 9-Benzylacridine, (I), the subject of this paper, is the precursor of the 10-methyl-9-benzylacridinium cation, which displays promising chemiluminogenic ability (McCapra *et al.*, 1977; Gagalis & Nikokavouras, 1979).

Table 1 lists the parameters characterizing the geometries of the central acridine ring system of (I) and its C9 substituent; they are typical for acridine-based derivatives (Leardini *et al.*, 1998; Mrozek *et al.*, 2002; Ebead *et al.*, 2005). With respective average deviations from planarity of 0.012 and 0.004 Å, the acridine system and phenyl ring in (I) are oriented at 73.3 (2)° to each other (Fig. 1).

In the monoclinic crystal structure of (I), molecules related by a centre of symmetry are arranged in pairs stabilized *via* π–π interactions between acridine units (Fig. 2 and Table 2). Adjacent pairs, with acridine ring systems arranged in a herringbone pattern, are linked through a network of C—H$\cdots\pi$ interactions (Fig. 2, Table 3), which cause the acridine systems, inclined to the *ab* plane at an angle 74.8 (2)°, to align themselves in layers. The crystal structure is stabilized by non-specific dispersive interactions between these layers. The acridine ring systems in pairs are parallel, whereas those in adjacent pairs are inclined to each other at 78.3 (2)°.

Analysis of the crystal structures of molecules in which –CH$_2$– has been replaced by –NH–, –O– or –S–, *i.e.* the compounds *N*-phenylacridin-9-amine, (II) (Leardini *et al.*, 1998), 9-phenoxyacridine, (III) (Ebead *et al.*, 2005), and 9-[2-methyl-4-nitrophenyl)thio]acridine, (IV) (Mrozek *et al.*, 2002), shows that the C9—C(N,O,S)15—C16 angles are 113.7 (2), 125.2 (2), 118.1 (2) and 103.5 (2)° for compounds (I)–(IV), respectively, while the angles between the acridine and benzene ring systems are 73.3 (2), 67.1 (2), 85.2 (2) and 74.1 (2)°, respectively.

In the crystal structures, the molecules of (I), (III) and (IV) form pairs that are stabilized *via* π–π interactions. Additional stabilization is provided by C—H$\cdots$N interactions, which are intramolecular in the case of (III) and intermolecular in the case of (IV). These pairs are linked through a network of C—H$\cdots\pi$ interactions in (I), C—H$\cdots$N and C—H$\cdots\pi$ interactions in (III), and π–π interactions in (IV). In the crystal structure of (II), the molecules are linked through a network of multidirectional N—H$\cdots$N, C—H$\cdots$N and C—H$\cdots\pi$ interactions. From this comparison, it is evident that the structural features of the compounds investigated display certain similarities, *e.g.* the mutual arrangement of the acridine and benzene ring systems or the formation of pairs, but also noticeable differences.

Experimental

The title compound was synthesized by treating *N*-phenylaniline with an equimolar amount of phenylacetic acid, both dispersed in molten zinc chloride (483 K, 24 h) (Huntress & Shaw, 1948). The crude product was purified by gravitational column chromatography (SiO$_2$, cyclohexane–ethyl acetate, 5:2 *v*/*v*). Pale-yellow crystals of (I) suitable for X-ray investigations were grown from absolute ethanol (m.p. 430–431 K).

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Crystal data

$C_{20}H_{15}N$
$M_r = 269.33$
Monoclinic, $P2_1/n$
$a = 10.713$ (2) Å
$b = 10.605$ (2) Å
$c = 13.033$ (3) Å
$\beta = 105.33$ (3)°

$V = 1428.0$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 290$ (2) K
0.4 × 0.3 × 0.2 mm

Data collection

Kuma KM-4 diffractometer
Absorption correction: none
2634 measured reflections
2517 independent reflections
1598 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.018$
3 standard reflections
every 200 reflections
intensity decay: 1.5%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.110$
$S = 1.05$
2517 reflections

191 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.14$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C9—C15	1.508 (2)	C15—C16	1.509 (2)
N10—C12	1.339 (2)		
C9—C15—C16	113.66 (13)	C12—N10—C14	117.67 (13)
C11—C9—C15	121.60 (15)		
C1—C11—C9—C15	1.8 (2)	C11—C9—C15—C16	96.03 (18)
C9—C15—C16—C17	126.50 (17)		

Table 2
π–π interactions (Å,°).

*Cg*1 is the centroid of ring C9/C11/C12/N10/C14/C13 and *Cg*2 is the centroid of ring C1–C4/C12/C11. *Cg*···*Cg* is the distance between ring centroids. The dihedral angle is that between the planes of the rings *CgI* and *CgJ*. The interplanar distance is the perpendicular distance of *CgI* from ring *J*. The offset is computed as the third side of the right-angled triangle involving the *Cg*···*Cg* distance and the interplanar distance, as defined above.

CgI	*CgJ*	*Cg*···*Cg*	Dihedral angle	Interplanar distance	Offset
1	2$^{\rm iii}$	3.665 (2)	1.0	3.378 (3)	1.422 (3)
2	1$^{\rm iii}$	3.665 (2)	1.0	3.403 (3)	1.361 (3)
2	2$^{\rm iii}$	3.865 (2)	0.0	3.392 (3)	1.853 (3)

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

Table 3
C—H···π interactions (Å, °).

X—H	*Cg*	H···*Cg*	*X*···*J*	*X*—*I*···*J*
C3—H3	3$^{\rm i}$	2.99	3.772 (2)	143
C7—H7	2$^{\rm ii}$	2.80	3.582 (2)	143

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$; (ii) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$. *Cg*2 is the centroid of ring C1–C4/C12/C11 and *Cg*3 is the centroid of the ring C5–C8/C13/C14.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *KM-4 Software* (Oxford Diffraction, 2003); cell refinement: *KM-4 Software*; data reduction: *KM-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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