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9-(4-Nitrophenyl)-9*H*-carbazole

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In the title compound, $C_{18}H_{12}N_2O_2$, the carbazole ring system is essentially planar and makes a dihedral angle of 53.08 (4)° with the plane of the nitrobenzene ring. In the crystal structure, inversion-related molecules form a C—H$\cdots$O hydrogen-bonded dimer.

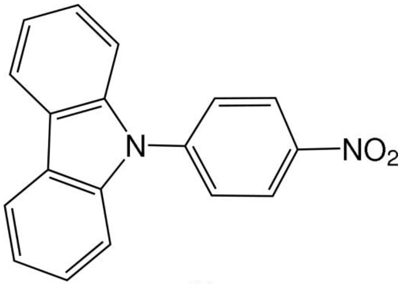
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 15.5

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

Comment

Carbazole-based compounds play a very important role in electroactive and photoactive materials (Morin *et al.*, 2004). In organic light-emitting diodes (OLEDs), carbazole derivatives are usually used as host materials for both small-molecule OLEDs (such as 4,4′-*N*,*N*′-dicarbazolebiphenyl, CBP) and polymer OLEDs [such as poly(vinylcarbazole), PVK] due to their high triplet energy and good hole-transporting and electron-blocking capability (Song *et al.*, 1999). The title compound, (I), emits blue luminescence both in the solid state and in organic solution upon irradiation by UV light at ambient temperature. Compound (I) is a useful intermediate, from which many carbazole derivatives with extended aromatic systems can be constructed.



(I)

The title molecule has approximate *C*2 symmetry. The carbazole ring system is essentially planar, with a mean deviation of 0.019 Å (Fig. 1). The dihedral angle between the C13–C18 benzene ring and the plane of the carbazole ring system is 53.08 (4)°. The C15—C16—N2—O2 [5.1 (2)°] and C17—C16—N2—O1 [6.2 (2)°] torsion angles indicate that the nitro group is twisted slightly away from the plane of the C13–C18 benzene ring. The C1—N1 and C12—N1 distances are smaller than the C13—N1 distance (Table 1). The C—N distance involving the N atom of the nitro group is longer than the C—N distances involving the carbazole N atom (Table 1).

In the crystal structure, centrosymmetrically related molecules are linked by C—H$\cdots$O intermolecular hydrogen bonds to form a dimer (Fig. 2).

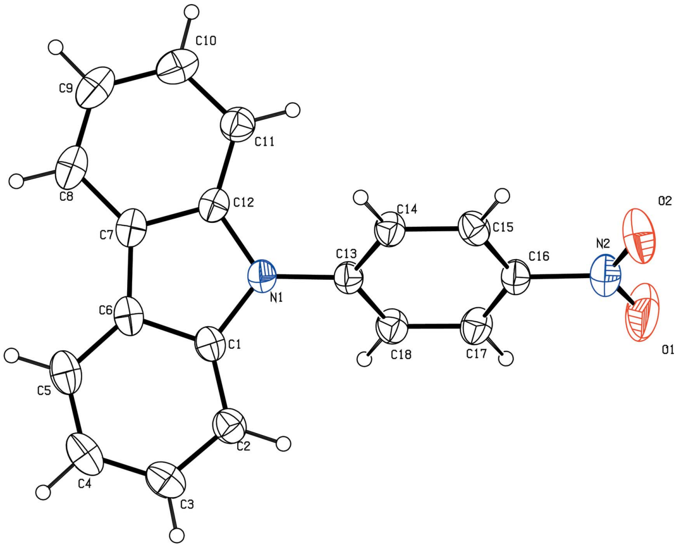


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

Carbazole and 1-nitrobenzene were purchased from Acros and used without further purification. Carbazole (0.5 mmol, 83.6 mg) and potassium hydroxide (5.0 mmol, 280.0 mg) were dissolved in 1-nitrobenzene (10 ml). The mixture was refluxed and stirred for 2 h to obtain a clear orange solution. After allowing the solution to stand in air for 8 d, yellow block-shaped crystals of (I) were formed by slow evaporation of the solvent. The crystals were isolated, washed with light petroleum and dried *in vacuo* (yield 85.8%; m.p = 483.3–484.2 K). Spectroscopic analysis: ^{1}H NMR (CDCl$_3$, δ, p.p.m.): 8.48 (*d*, J = 8.7 Hz, 2H), 8.15 (*d*, J = 7.8 Hz, 2H), 7.80 (*d*, J = 8.7 Hz, 2H), 7.45 (*m*, 4H) 7.35 (*t*, J = 6.6 Hz, 2H).

Crystal data

$C_{18}H_{12}N_2O_2$
$M_r = 288.30$
Monoclinic, $P2_1/c$
$a = 8.356$ (2) Å
$b = 21.620$ (5) Å
$c = 8.153$ (2) Å
$\beta = 105.592$ (4)°
$V = 1418.7$ (6) Å^3
$Z = 4$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2691 reflections
$\theta = 2.2$–25.6°
$\mu = 0.09$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.34 × 0.20 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.970$, $T_{max} = 0.986$
9337 measured reflections
3079 independent reflections
2132 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.0°$
$h = -10 \rightarrow 10$
$k = -25 \rightarrow 27$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.120$
$S = 0.96$
3079 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

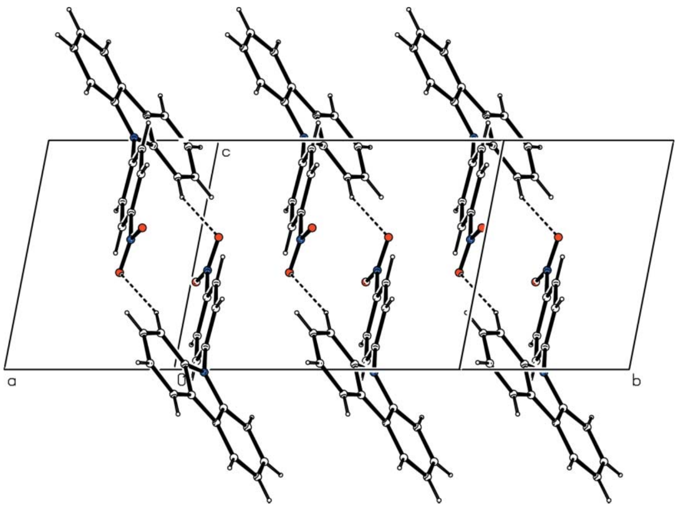


Figure 2
Part of the crystal packing of (I), showing C—H···O hydrogen-bonded dimers. Hydrogen bonds are shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.4004 (18)	C16—N2	1.4692 (18)
C12—N1	1.4037 (18)	N2—O2	1.2086 (17)
C13—N1	1.4181 (16)	N2—O1	1.2123 (18)
C1—N1—C12	108.52 (11)	O2—N2—O1	123.10 (14)
C1—N1—C13	126.25 (11)	O2—N2—C16	118.63 (14)
C12—N1—C13	125.13 (11)	O1—N2—C16	118.26 (15)
C14—C13—N1—C1	−126.76 (15)	C18—C13—N1—C12	−130.22 (14)
C18—C13—N1—C1	53.81 (19)	C17—C16—N2—O2	−175.13 (14)
C14—C13—N1—C12	49.21 (18)	C15—C16—N2—O1	−173.49 (15)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O2^i	0.93	2.52	3.396 (2)	157

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

H atoms were placed in idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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