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2-Cyano-*N*-(diphenylmethylene)benzenamine

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Key indicators

Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.139
Data-to-parameter ratio = 18.1

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

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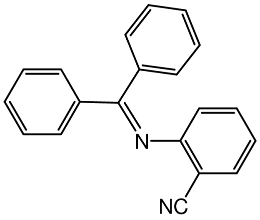
In the title compound, $C_{20}H_{14}N_2$, the orientations of the three aromatic rings are determined by the sp^2 state of the two central N and C atoms. The crystal packing of the title compound is stabilized by weak C—H···π interactions.

Comment

Photo-induced electron transfer (PET) reactions of nitroaromatic compounds with diphenylacetylenes have been extensively investigated (Scheinbaum, 1964; Tian & Xu, 2002). These reactions afford routes to benzenamine derivatives whose structures have been reported in our previous studies (Tian *et al.*, 2002; Zhang *et al.*, 2002; Usman *et al.*, 2002*a*,*b*,*c*). In our ongoing study of the PET reactions of nitroaromatic compounds, we have carried out a similar reaction for 2-nitrobenzonitrile with an excess amount of 1,2-diphenylacetylene in benzene, and isolated the title compound, (I). An X-ray crystal structure of (I) was undertaken to elucidate its molecular conformation.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and are comparable with those in the related compound 3-[(diphenylmethylene)amino]phthalonitrile (Tian *et al.*, 2002). The C19—C20 bond [1.443 (4) Å] is elongated compared with that of a typical Csp^2—Csp^1 bond, but this bond distance is within the acceptable range compared with those in other benzenecarbonitrile derivatives [1.444 (7) Å (Toupet *et al.*, 1989), 1.445 (4) Å (Zhang *et al.*, 2002) and 1.441 (3) Å (Tian *et al.*, 2002)].

The iminoaromatic moiety is nearly planar, with atom N1 displaced by 0.048 (2) Å from the aromatic plane. The dihedral angles between this aromatic plane and the C1—C6 and C8—C13 phenyl rings are 67.1 (1) and 59.5 (1)°, respectively. The two phenyl rings make a dihedral angle of 71.8 (1) Å with respect to each other. The C6—C7—C8 angle joining the two phenyl rings is 117.8 (2)°, which is comparable with the corresponding value in a related structure [117.3 (2)°; Tian *et al.*, 2002]. Atoms N1, C6, C7 and C8, linking the three aromatic rings, are Csp^2 in character, with the C14—N1—C7—C6 and C14—N1—C7—C8 torsion angles being 179.5 (2) and 3.9 (3)°, respectively.

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The molecular packing is stabilized by weak C—H$\cdots\pi$ interactions involving atoms C12 and C15 and the C14–C19 and C1–C6 aromatic rings [Table 2; $Cg(A)$ and $Cg(B)$ denote the centroids of the C14–C19 and C1–C6 rings, respectively].

Experimental

The title compound was prepared by the photoinduced reaction of 2-nitrobenzene with 1,2-diphenylacetylene in benzene and was isolated fromthe reaction mixture using silica-gel column chromatography. Single crystals were obtained by slow evaporation of a petroleum ether–ethyl acetate solution.

Crystal data

$C_{20}H_{14}N_2$
$M_r = 282.33$
Monoclinic, $P2_1/c$
$a = 9.3429$ (3) Å
$b = 15.8543$ (2) Å
$c = 10.6022$ (3) Å
$\beta = 104.45$ (3)°
$V = 1520.8$ (2) Å^3
$Z = 4$
$D_x = 1.233$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2721 reflections
$\theta = 2.6$–28.3°
$\mu = 0.07$ mm^{-1}
$T = 213$ (2) K
Slab, colorless
0.32 × 0.22 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
8637 measured reflections
3625 independent reflections
1539 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.102$
$\theta_{\rm max} = 28.3$°
$h = -12 \rightarrow 12$
$k = -20 \rightarrow 16$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.139$
$S = 0.81$
3625 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.24$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.038 (3)

Table 1
Selected interatomic (Å,).

N1—C7	1.280 (2)	C6—C7	1.496 (3)
N1—C14	1.420 (3)	C7—C8	1.498 (3)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C12—H12$\cdots Cg(A^{\rm i})$	0.93	2.89	3.801 (2)	165
C15—H15$\cdots Cg(B^{\rm ii})$	0.93	2.77	3.552 (2)	142

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

The H atoms were positioned geometrically and treated as riding atoms, with $U_{\rm iso}({\rm H}) = 1.2\,U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

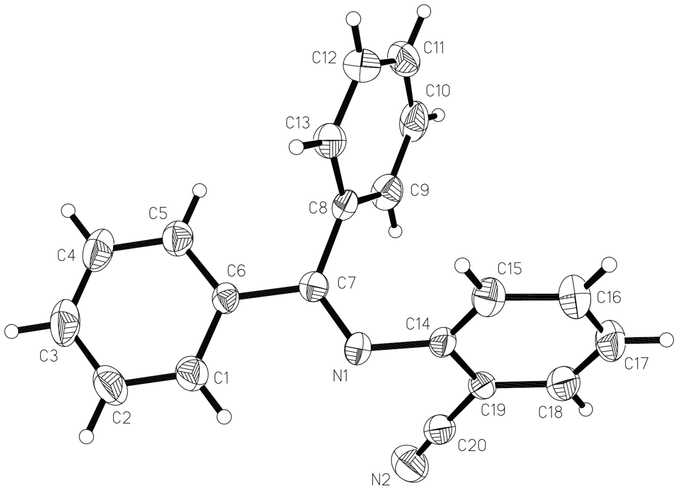

Figure 1
A view of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms as small spheres of arbitrary radii.

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