

4-[(*E*)-Phenyliminomethyl]benzonitrile

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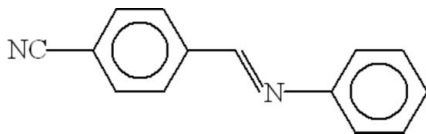
Received 29 March 2008; accepted 31 March 2008

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.047; wR factor = 0.119; data-to-parameter ratio = 16.4.

In the molecule of the title compound, $\text{C}_{14}\text{H}_{10}\text{N}_2$, the two aromatic rings are oriented at a dihedral angle of $32.22(6)^\circ$. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into centrosymmetric $R_2^2(10)$ dimers. A weak $\pi-\pi$ interaction between the cyanobenzene rings, with a centroid-centroid distance of $3.8447(3)$ Å, further stabilizes the crystal structure. There is also a $\text{C}-\text{H}\cdots\pi$ interaction between the aniline ring and a CH group of the cyanobenzene ring.

Related literature

For related structures, see: Ojala *et al.* (2002). For ring motif details, see: Bernstein *et al.* (1995); Etter (1990). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{10}\text{N}_2$

$M_r = 206.24$

Monoclinic, $P2_1/n$

$a = 7.2673(4)$ Å

$b = 10.0287(7)$ Å

$c = 15.4306(12)$ Å

$\beta = 96.177(2)^\circ$

$V = 1118.08(13)$ Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 0.07$ mm⁻¹

$T = 296(2)$ K

$0.20 \times 0.15 \times 0.12$ mm

Data collection

Bruker Kappa-APEXII CCD
 diffractometer

Absorption correction: multi-scan
 (SADABS; Bruker, 2005)

$T_{\min} = 0.983$, $T_{\max} = 0.994$

13128 measured reflections

2883 independent reflections

1423 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.118$

$S = 1.03$

2883 reflections

176 parameters

All H-atom parameters refined

$\Delta\rho_{\text{max}} = 0.13$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.10$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{N2}^i$	0.980 (13)	2.616 (14)	3.473 (2)	146.1 (10)
$\text{C5}-\text{H5}\cdots\text{Cg}^{ii}$	0.975 (13)	2.650 (14)	3.5970 (17)	163.9 (11)

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$. Cg is the centroid of atoms C9–C14.

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2; data reduction: SAINT (Bruker, 2007); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the Higher Education Commission, Islamabad, Pakistan, for funding the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2445).

References

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supplementary materials

Acta Cryst. (2008). E64, o790 [doi:10.1107/S1600536808008672]

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Comment

The crystal structures of *p*-halo-*N*-(*p*-cyanobenzylidene)-aniline and *p*-cyano-*N*-(*p*-halobenzylidene)aniline, (halo = bromo and chloro) (Ojala *et al.*, 2002) have been reported, previously. The title compound, (I), differs due to no attachment of halogen atoms. It is prepared in aqueous medium and we report herein its crystal structure.

The molecule of (I), (Fig. 1), is a Schiff base ligand of aniline and *p*-cyanobenzaldehyde. The bond lengths (Allen *et al.*, 1987) and angles are generally within normal ranges. Rings A (C1-C6) and B (C9-C14) are, of course, planar, and they are oriented at a dihedral angle of 32.22 (6)°.

In the crystal structure, intermolecular C-H...N hydrogen bonds (Table 1) link the molecules into centrosymmetric $R_2^2(10)$ dimers (Fig. 2) (Bernstein *et al.*, 1995; Etter, 1990), in which they may be effective in the stabilization of the structure. A weak $\pi\cdots\pi$ interaction between the A rings, at x, y, z and $1-x, 1-y, -z$, further stabilizes the structure, with a centroid-centroid distance of 3.8447 (3) Å. There is also a C—H... π interaction between the ring B at $x - 1/2, 1/2 - y, z - 1/2$ and C5-H5, with H5-centroid distance of 2.650 (14) Å.

Experimental

The starting materials employed were first purified by distillation or crystallization just before use. The experiment was performed in stoppered flask at room temperature. The title compound was synthesized by using equimolar mixture of aniline (5 mmol) and *p*-cyanobenzaldehyde (5 mmol) of pH = 9 in aqueous medium. The product was precipitated after a few minutes, and separated by filtration, washed with a small amount of water and dried for 2 d at room temperature in a vacuum desiccator. The dried filtrate was used for X-ray analysis (yield; 53.09%, m.p. 339 K).

Refinement

H atoms were located in a difference syntheses and refined [C-H = 0.949 (15)-0.999 (12) Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

Figures

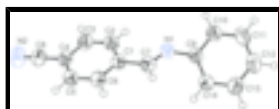


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

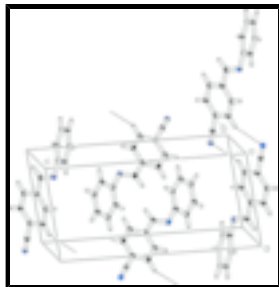


Fig. 2. A partial packing diagram of (I), showing the formation of centro-symmetric $R_2^2(10)$ ring motifs. Hydrogen bonds are shown as dashed lines.

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$C_{14}H_{10}N_2$

$M_r = 206.24$

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Hall symbol: $-P\ 2_1/n$

$a = 7.2673$ (4) Å

$b = 10.0287$ (7) Å

$c = 15.4306$ (12) Å

$\beta = 96.177$ (2)°

$V = 1118.08$ (13) Å³

$Z = 4$

$F_{000} = 432$

$D_x = 1.226$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2883 reflections

$\theta = 2.4$ – 28.7 °

$\mu = 0.07$ mm⁻¹

$T = 296$ (2) K

Prismatic, yellow

$0.20 \times 0.15 \times 0.12$ mm

Data collection

Bruker Kappa-APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 7.30 pixels mm⁻¹

$T = 296$ (2) K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{\min} = 0.983$, $T_{\max} = 0.994$

13128 measured reflections

2883 independent reflections

1423 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 28.7$ °

$\theta_{\min} = 2.4$ °

$h = -9 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.118$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.03$ $(\Delta/\sigma)_{\max} < 0.001$
 2883 reflections $\Delta\rho_{\max} = 0.13 \text{ e } \text{\AA}^{-3}$
 176 parameters $\Delta\rho_{\min} = -0.10 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.70615 (14)	0.08086 (11)	0.10666 (8)	0.0518 (3)
N2	0.05182 (19)	0.57458 (14)	-0.13327 (10)	0.0855 (5)
C1	0.57569 (17)	0.23345 (13)	-0.00193 (9)	0.0462 (4)
C2	0.40486 (19)	0.23930 (15)	0.03050 (10)	0.0559 (4)
H2	0.3870 (17)	0.1816 (14)	0.0777 (9)	0.067*
C3	0.27073 (19)	0.32560 (16)	-0.00409 (10)	0.0593 (4)
H3	0.1494 (18)	0.3263 (13)	0.0181 (9)	0.071*
C4	0.30456 (17)	0.40866 (13)	-0.07259 (9)	0.0493 (4)
C5	0.4727 (2)	0.40351 (15)	-0.10663 (10)	0.0538 (4)
H5	0.4929 (16)	0.4628 (13)	-0.1547 (9)	0.065*
C6	0.60682 (19)	0.31589 (15)	-0.07083 (10)	0.0528 (4)
H6	0.7273 (17)	0.3117 (13)	-0.0919 (9)	0.063*
C7	0.72303 (19)	0.14630 (14)	0.03760 (10)	0.0519 (4)
H7	0.8385 (17)	0.1419 (12)	0.0080 (8)	0.062*
C8	0.1639 (2)	0.50057 (16)	-0.10713 (10)	0.0610 (4)
C9	0.85826 (18)	0.00574 (13)	0.14575 (9)	0.0476 (4)
C10	0.8196 (2)	-0.11183 (15)	0.18708 (10)	0.0569 (4)
H10	0.6901 (18)	-0.1361 (13)	0.1860 (9)	0.068*
C11	0.9612 (2)	-0.18768 (16)	0.22793 (10)	0.0657 (5)
H11	0.9274 (18)	-0.2675 (15)	0.2552 (10)	0.079*
C12	1.1415 (2)	-0.14576 (17)	0.22995 (11)	0.0668 (5)
H12	1.2406 (18)	-0.1973 (15)	0.2609 (10)	0.080*
C13	1.1803 (2)	-0.02736 (18)	0.19159 (11)	0.0684 (5)
H13	1.305 (2)	0.0051 (15)	0.1918 (9)	0.082*
C14	1.03990 (19)	0.04859 (16)	0.14922 (11)	0.0605 (4)
H14	1.0655 (18)	0.1354 (14)	0.1248 (9)	0.073*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0550 (7)	0.0462 (7)	0.0531 (8)	0.0004 (5)	0.0010 (6)	0.0009 (6)
N2	0.0759 (9)	0.0934 (11)	0.0861 (11)	0.0287 (9)	0.0031 (8)	0.0113 (9)
C1	0.0490 (8)	0.0449 (8)	0.0445 (9)	0.0007 (6)	0.0040 (7)	-0.0042 (7)
C2	0.0552 (8)	0.0586 (10)	0.0550 (11)	-0.0002 (8)	0.0104 (8)	0.0092 (8)
C3	0.0482 (8)	0.0703 (11)	0.0606 (11)	0.0040 (8)	0.0109 (8)	0.0044 (9)
C4	0.0509 (8)	0.0485 (9)	0.0473 (9)	0.0033 (7)	-0.0005 (7)	-0.0045 (7)
C5	0.0621 (9)	0.0525 (9)	0.0470 (10)	0.0015 (7)	0.0070 (8)	0.0037 (7)
C6	0.0511 (8)	0.0595 (10)	0.0490 (10)	0.0035 (8)	0.0102 (7)	0.0008 (8)
C7	0.0531 (8)	0.0507 (9)	0.0518 (10)	0.0023 (7)	0.0060 (7)	-0.0034 (8)
C8	0.0597 (9)	0.0658 (11)	0.0571 (11)	0.0072 (9)	0.0036 (8)	-0.0016 (9)
C9	0.0559 (8)	0.0414 (8)	0.0447 (9)	0.0025 (7)	0.0024 (7)	-0.0017 (7)
C10	0.0656 (9)	0.0498 (9)	0.0535 (10)	-0.0058 (8)	-0.0024 (8)	0.0003 (8)
C11	0.0921 (12)	0.0461 (10)	0.0556 (11)	-0.0021 (9)	-0.0072 (9)	0.0045 (8)
C12	0.0790 (12)	0.0624 (11)	0.0565 (11)	0.0186 (9)	-0.0047 (9)	0.0014 (9)
C13	0.0580 (9)	0.0749 (12)	0.0718 (12)	0.0052 (9)	0.0051 (9)	0.0107 (10)
C14	0.0570 (9)	0.0559 (9)	0.0682 (12)	0.0006 (8)	0.0046 (8)	0.0136 (9)

Geometric parameters (\AA , $^\circ$)

N1—C7	1.2686 (17)	C6—H6	0.967 (12)
N1—C9	1.4177 (16)	C7—H7	0.999 (12)
N2—C8	1.1429 (17)	C9—C10	1.3835 (18)
C1—C6	1.3845 (19)	C9—C14	1.3838 (18)
C1—C2	1.3888 (17)	C10—C11	1.376 (2)
C1—C7	1.4635 (18)	C10—H10	0.971 (12)
C2—C3	1.3683 (19)	C11—C12	1.373 (2)
C2—H2	0.950 (14)	C11—H11	0.949 (15)
C3—C4	1.3883 (19)	C12—C13	1.370 (2)
C3—H3	0.979 (13)	C12—H12	0.970 (14)
C4—C5	1.3823 (19)	C13—C14	1.3801 (19)
C4—C8	1.436 (2)	C13—H13	0.965 (14)
C5—C6	1.3823 (19)	C14—H14	0.975 (14)
C5—H5	0.975 (13)		
C7—N1—C9	119.40 (12)	C1—C7—H7	116.7 (8)
C6—C1—C2	118.54 (13)	N2—C8—C4	178.87 (17)
C6—C1—C7	120.26 (12)	C10—C9—C14	119.13 (13)
C2—C1—C7	121.16 (13)	C10—C9—N1	117.48 (12)
C3—C2—C1	120.87 (14)	C14—C9—N1	123.25 (13)
C3—C2—H2	122.3 (8)	C11—C10—C9	120.22 (14)
C1—C2—H2	116.8 (8)	C11—C10—H10	123.0 (8)
C2—C3—C4	119.97 (14)	C9—C10—H10	116.8 (8)
C2—C3—H3	119.9 (8)	C12—C11—C10	120.37 (16)
C4—C3—H3	120.1 (8)	C12—C11—H11	122.7 (9)
C5—C4—C3	120.20 (13)	C10—C11—H11	116.9 (9)

C5—C4—C8	120.42 (13)	C13—C12—C11	119.72 (16)
C3—C4—C8	119.37 (13)	C13—C12—H12	119.9 (8)
C6—C5—C4	119.08 (14)	C11—C12—H12	120.3 (8)
C6—C5—H5	122.3 (7)	C12—C13—C14	120.48 (16)
C4—C5—H5	118.6 (7)	C12—C13—H13	121.9 (9)
C5—C6—C1	121.34 (14)	C14—C13—H13	117.6 (9)
C5—C6—H6	121.2 (8)	C13—C14—C9	120.02 (14)
C1—C6—H6	117.5 (8)	C13—C14—H14	121.0 (8)
N1—C7—C1	121.76 (13)	C9—C14—H14	118.9 (8)
N1—C7—H7	121.6 (7)		
C6—C1—C2—C3	-0.7 (2)	C2—C1—C7—N1	-5.6 (2)
C7—C1—C2—C3	176.87 (14)	C7—N1—C9—C10	-146.46 (13)
C1—C2—C3—C4	0.1 (2)	C7—N1—C9—C14	37.8 (2)
C2—C3—C4—C5	0.7 (2)	C14—C9—C10—C11	-2.7 (2)
C2—C3—C4—C8	-178.79 (13)	N1—C9—C10—C11	-178.56 (14)
C3—C4—C5—C6	-0.8 (2)	C9—C10—C11—C12	1.6 (2)
C8—C4—C5—C6	178.69 (13)	C10—C11—C12—C13	0.5 (3)
C4—C5—C6—C1	0.1 (2)	C11—C12—C13—C14	-1.5 (3)
C2—C1—C6—C5	0.6 (2)	C12—C13—C14—C9	0.4 (3)
C7—C1—C6—C5	-176.99 (12)	C10—C9—C14—C13	1.6 (2)
C9—N1—C7—C1	-175.33 (11)	N1—C9—C14—C13	177.28 (14)
C6—C1—C7—N1	172.00 (13)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3 \cdots N2 ⁱ	0.980 (13)	2.616 (14)	3.473 (2)	146.1 (10)
C5—H5 \cdots Cg ⁱⁱ	0.975 (13)	2.650 (14)	3.5970 (17)	163.9 (11)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $x-1/2, -y+1/2, z-1/2$.

Fig. 1

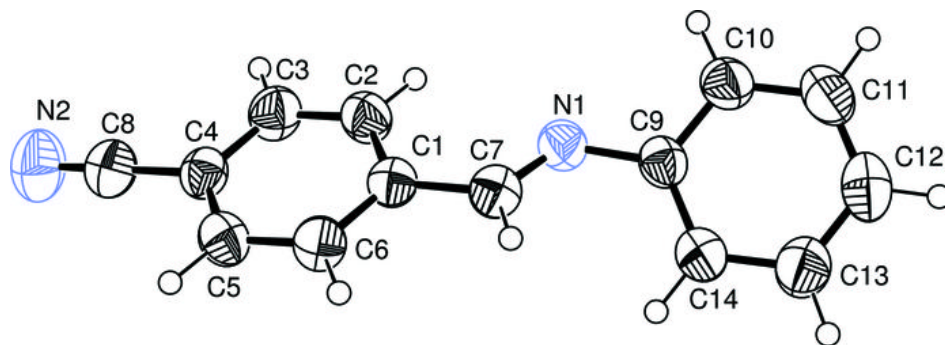


Fig. 2

