Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(Benzylideneamino)pyridinium iodide

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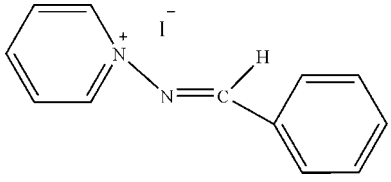
Received 18 December 2008; accepted 23 December 2008

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.030; wR factor = 0.075; data-to-parameter ratio = 15.7.

In the title compound, $C_{12}H_{11}N_2^+\cdot I^-$, the aromatic rings are oriented at a dihedral angle of 73.40 (3)°. In the crystal structure, π–π contacts between the pyridine rings and the benzene and pyridine rings [centroid–centroid distances = 3.548 (3) and 4.211 (3) Å] may stabilize the structure.

Related literature

For background, see: Okamoto *et al.* (1967). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{12}H_{11}N_2^+\cdot I^-$
M_r = 310.13
Monoclinic, $P2_1/c$
a = 10.5722 (17) Å
b = 7.8219 (13) Å
c = 15.386 (3) Å
β = 108.354 (2)°
V = 1207.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.62 mm^{-1}
T = 291 (2) K
0.13 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.727, T_{max} = 0.780
5768 measured reflections
2133 independent reflections
1713 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 0.94
2133 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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); software used to prepare material for publication: *SHELXL97*.

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2601).

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supporting information

Acta Cryst. (2009). E**65**, o229 [doi:10.1107/S1600536808043717]

1-(Benzylideneamino)pyridinum iodide

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S1. Comment

Some derivatives of 1-aminopyidium iodide are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (N1/C1-C5) and B (C7-C12) are, of course, planar, and they are oriented at a dihedral angle of 73.40 (3)°.

In the crystal structure, π-π contacts between the pyridine and the benzene rings and the pyridine rings, Cg1—Cg2^{i} and Cg1—Cg1^{ii} [symmetry codes: (i) x, 3/2 - y, z - 1/2; (ii) 1 - x, 2 - y, -z, where Cg1 and Cg2 are centroids of the rings A (N1/C1-C5) and B (C7-C12) , respectively] may stabilize the structure, with centroid-centroid distances of 3.548 (3) Å and 4.211 (3) Å.

S2. Experimental

For the preparation of the title compound, 1-aminopyridinium iodide (22.2 g, 0.10 mol) was dissolved in ethanol (20 ml), benzaldehyde(10.6 g, 0.10 mol) was added with stirring, and then the mixture was heated at reflux for 5 h. Upon cooling to room temperature, a precipitate formed, which was collected by filtration and washed with cold ethanol (2 X 10 ml) to obtain a yellow solid (yield; 21.7 g, 70%). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93 Å for aromatic and methine H and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

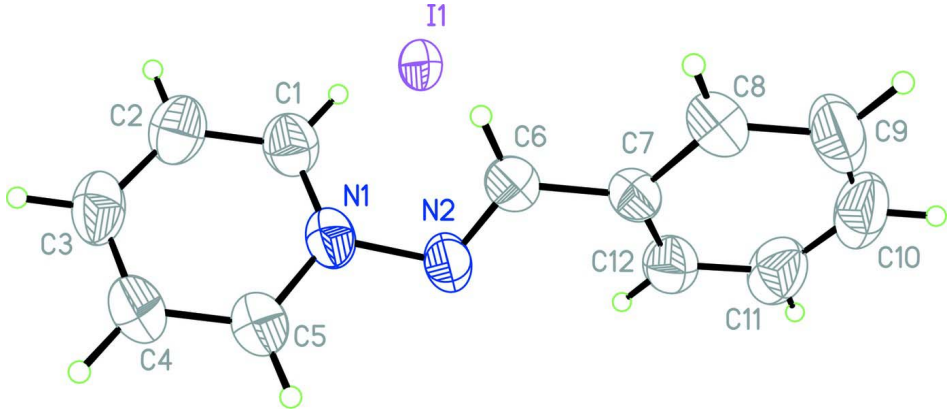

Figure 1

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

1-(Benzylideneamino)pyridinium iodide

Crystal data

$C_{12}H_{11}N_2^+ \cdot I^-$
$M_r = 310.13$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.5722\ (17)$ Å
$b = 7.8219\ (13)$ Å
$c = 15.386\ (3)$ Å
$\beta = 108.354\ (2)°$
$V = 1207.6\ (4)$ Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.706$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 2.1–25.3°$
$\mu = 2.62$ mm^{-1}
$T = 291$ K
Block, yellow
0.13 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.727$, $T_{max} = 0.780$
5768 measured reflections
2133 independent reflections
1713 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -12 \rightarrow 12$
$k = -9 \rightarrow 7$
$l = -18 \rightarrow 18$
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.075$
$S = 0.94$
2133 reflections
136 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
I1	0.36542 (2)	0.37261 (3)	0.175113 (16)	0.05509 (13)
N1	0.2501 (3)	0.8944 (3)	0.03899 (19)	0.0462 (7)
N2	0.1744 (3)	0.8956 (3)	0.10105 (19)	0.0482 (7)

C1	0.3602 (4)	0.7989 (5)	0.0544 (3)	0.0543 (9)
H1	0.3942	0.7393	0.1091	0.065*
C2	0.4222 (4)	0.7904 (5)	−0.0117 (3)	0.0597 (10)
H2	0.4975	0.7225	−0.0024	0.072*
C3	0.3734 (4)	0.8812 (5)	−0.0909 (3)	0.0586 (10)
H3	0.4162	0.8775	−0.1353	0.070*
C4	0.2612 (4)	0.9776 (6)	−0.1045 (2)	0.0633 (10)
H4	0.2274	1.0402	−0.1582	0.076*
C5	0.1982 (4)	0.9821 (5)	−0.0388 (2)	0.0617 (10)
H5	0.1205	1.0454	−0.0484	0.074*
C6	0.2447 (3)	0.9324 (4)	0.1829 (2)	0.0439 (8)
H6	0.3347	0.9579	0.1961	0.053*
C7	0.1831 (3)	0.9341 (5)	0.2553 (2)	0.0447 (8)
C8	0.2456 (4)	1.0226 (5)	0.3354 (2)	0.0584 (9)
H8	0.3250	1.0802	0.3419	0.070*
C9	0.0654 (4)	0.8452 (5)	0.2465 (3)	0.0566 (10)
H9	0.0240	0.7838	0.1934	0.068*
C10	0.0110 (4)	0.8488 (5)	0.3166 (3)	0.0687 (12)
H10	−0.0678	0.7902	0.3109	0.082*
C11	0.0729 (5)	0.9391 (6)	0.3955 (3)	0.0748 (13)
H11	0.0352	0.9419	0.4425	0.090*
C12	0.1899 (5)	1.0252 (6)	0.4051 (3)	0.0716 (12)
H12	0.2315	1.0851	0.4588	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.05786 (18)	0.0622 (2)	0.04976 (17)	−0.00118 (11)	0.02344 (12)	0.00535 (11)
N1	0.0537 (16)	0.0507 (17)	0.0363 (15)	−0.0039 (13)	0.0172 (13)	−0.0040 (13)
N2	0.0509 (16)	0.0610 (18)	0.0355 (15)	−0.0047 (13)	0.0176 (13)	−0.0016 (14)
C1	0.064 (2)	0.050 (2)	0.052 (2)	0.0022 (18)	0.0222 (18)	0.0048 (18)
C2	0.066 (2)	0.055 (2)	0.067 (3)	0.0024 (19)	0.034 (2)	−0.005 (2)
C3	0.069 (2)	0.066 (2)	0.050 (2)	−0.012 (2)	0.0314 (19)	−0.013 (2)
C4	0.067 (2)	0.082 (3)	0.0402 (19)	0.001 (2)	0.0172 (18)	0.010 (2)
C5	0.061 (2)	0.083 (3)	0.043 (2)	0.010 (2)	0.0183 (17)	0.004 (2)
C6	0.0466 (18)	0.0441 (19)	0.0398 (19)	0.0008 (14)	0.0118 (15)	0.0004 (15)
C7	0.0471 (19)	0.0505 (19)	0.0351 (18)	0.0047 (15)	0.0107 (15)	0.0027 (16)
C8	0.061 (2)	0.070 (3)	0.0405 (19)	0.0007 (19)	0.0111 (17)	−0.0024 (19)
C9	0.054 (2)	0.068 (3)	0.050 (2)	−0.0020 (17)	0.0190 (18)	0.0039 (18)
C10	0.067 (3)	0.078 (3)	0.074 (3)	0.003 (2)	0.040 (2)	0.012 (2)
C11	0.097 (3)	0.082 (3)	0.062 (3)	0.033 (3)	0.049 (3)	0.019 (3)
C12	0.098 (3)	0.078 (3)	0.039 (2)	0.015 (3)	0.022 (2)	−0.004 (2)

Geometric parameters (Å, º)

N1—N2	1.426 (4)	C6—C7	1.457 (4)
C1—N1	1.340 (4)	C6—H6	0.9300
C1—C2	1.375 (5)	C7—C8	1.385 (5)

C1—H1	0.9300	C7—C9	1.394 (5)
C2—C3	1.364 (5)	C8—C12	1.377 (5)
C2—H2	0.9300	C8—H8	0.9300
C3—C4	1.365 (5)	C9—C10	1.374 (6)
C3—H3	0.9300	C9—H9	0.9300
C4—C5	1.374 (5)	C10—C11	1.378 (7)
C4—H4	0.9300	C10—H10	0.9300
C5—N1	1.339 (4)	C11—C12	1.375 (6)
C5—H5	0.9300	C11—H11	0.9300
C6—N2	1.277 (4)	C12—H12	0.9300
C5—N1—C1	122.2 (3)	N2—C6—H6	120.2
C5—N1—N2	116.0 (3)	C7—C6—H6	120.2
C1—N1—N2	121.6 (3)	C8—C7—C9	119.8 (3)
C6—N2—N1	112.8 (3)	C8—C7—C6	118.8 (3)
N1—C1—C2	119.1 (4)	C9—C7—C6	121.4 (3)
N1—C1—H1	120.4	C12—C8—C7	120.0 (4)
C2—C1—H1	120.4	C12—C8—H8	120.0
C3—C2—C1	120.1 (4)	C7—C8—H8	120.0
C3—C2—H2	119.9	C10—C9—C7	119.7 (4)
C1—C2—H2	119.9	C10—C9—H9	120.1
C2—C3—C4	119.3 (4)	C7—C9—H9	120.1
C2—C3—H3	120.3	C9—C10—C11	120.1 (4)
C4—C3—H3	120.3	C9—C10—H10	120.0
C3—C4—C5	120.1 (4)	C11—C10—H10	120.0
C3—C4—H4	119.9	C12—C11—C10	120.5 (4)
C5—C4—H4	119.9	C12—C11—H11	119.7
N1—C5—C4	119.2 (4)	C10—C11—H11	119.7
N1—C5—H5	120.4	C11—C12—C8	119.9 (4)
C4—C5—H5	120.4	C11—C12—H12	120.0
N2—C6—C7	119.7 (3)	C8—C12—H12	120.0