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4-Iodo-2,6-dimethylaniline

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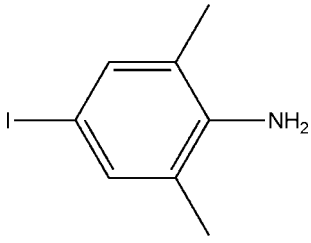
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.016 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 11.1.

In the molecule of the title compound, $C_8H_{10}IN$, the I, N and methyl C atoms lie in the benzene ring plane. In the crystal structure, intermolecular N—H···N hydrogen bonds may be effective in stabilizing the structure.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Zielinska & Skulski (2005); Glidewell *et al.* (2002).



Experimental

Crystal data

$C_8H_{10}IN$
M_r = 247.07
Orthorhombic, $P2_12_12_1$
a = 4.841 (1) Å
b = 11.389 (2) Å
c = 16.128 (3) Å
V = 889.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.53 mm^{-1}
T = 298 (2) K
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.306, T_{max} = 0.496
1036 measured reflections
1036 independent reflections
867 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.00
1036 reflections
93 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: 0.16 (13)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···N^{i}	0.86	2.45	3.248 (12)	155

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2285).

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supplementary materials

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4-Iodo-2,6-dimethylaniline

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Comment

The title compound, (I), contains amino and halogen groups, in which they can react with different groups to prepare various functional organic compounds. It is a kind of aromatic organic intermediate that can be used for many fields such as aromatic conductive polymers, organometallic chemistry *etc*. (Zielinska & Skulski, 2005). We herein report its crystal structure.

In the molecule of (I), (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987), which can be compared with the corresponding values in 2-iodo-*N*-(3-nitrobenzyl)aniline (Glidewell *et al.*, 2002). The atoms I, N and methyl carbons lie in the benzene ring plane.

In the crystal structure, intermolecular N—H···N hydrogen bonds (Table 2) may be effective in the stabilization of the structure, the molecules are stacked along the *a* axis (Fig. 2).

Experimental

The title compound, (I) was prepared by the literature method (Zielinska & Skulski, 2005). The crystals were obtained by dissolving (I) (0.5 g) in hexane (20 ml) and evaporating the solvent slowly at room temperature for about 7 d.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH_2) and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

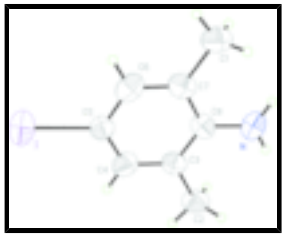

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

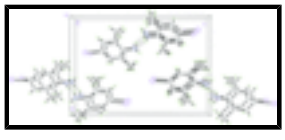

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

4-iodo-2,6-dimethylaniline

Crystal data

$C_8H_{10}IN$	$D_x = 1.846$ Mg m^{-3}
$M_r = 247.07$	Melting point: 324 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 25 reflections
$a = 4.841$ (1) Å	$\theta = 10$–13^o
$b = 11.389$ (2) Å	$\mu = 3.53$ mm^{-1}
$c = 16.128$ (3) Å	$T = 298$ (2) K
$V = 889.2$ (3) Å^3	Needle, white
$Z = 4$	0.40 × 0.20 × 0.20 mm
$F_{000} = 472$	

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.0000$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.9^o$
Monochromator: graphite	$\theta_{min} = 2.2^o$
$T = 298(2)$ K	$h = 0 \rightarrow 5$
$\omega/2\theta$ scans	$k = 0 \rightarrow 14$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 19$
$T_{min} = 0.306$, $T_{max} = 0.496$	3 standard reflections
1036 measured reflections	every 120 min
1036 independent reflections	intensity decay: 1%
867 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 4P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.144$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.62$ e Å^{-3}
1036 reflections	$\Delta\rho_{min} = -0.89$ e Å^{-3}
93 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), no Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.16 (13)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
I	0.9368 (2)	0.13850 (9)	0.90849 (5)	0.0746 (4)
N	1.380 (2)	0.1794 (9)	0.5450 (6)	0.056 (3)
H0A	1.4925	0.2344	0.5312	0.067*
H0B	1.3201	0.1311	0.5081	0.067*
C1	0.982 (3)	−0.0018 (11)	0.5800 (8)	0.069 (4)
H1A	0.9108	0.0430	0.5344	0.103*
H1B	0.8381	−0.0499	0.6027	0.103*
H1C	1.1303	−0.0510	0.5609	0.103*
C2	1.602 (3)	0.3380 (10)	0.6666 (8)	0.054 (3)
H2A	1.5346	0.3866	0.6224	0.081*
H2B	1.7700	0.3002	0.6496	0.081*
H2C	1.6372	0.3855	0.7146	0.081*
C3	1.385 (2)	0.2443 (8)	0.6879 (7)	0.041 (2)
C4	1.286 (3)	0.2360 (10)	0.7675 (7)	0.050 (3)
H4A	1.3503	0.2874	0.8079	0.060*
C5	1.095 (3)	0.1533 (9)	0.7877 (6)	0.045 (2)
C6	0.994 (2)	0.0768 (11)	0.7285 (7)	0.056 (3)
H6A	0.8615	0.0215	0.7429	0.067*
C7	1.092 (3)	0.0824 (9)	0.6476 (6)	0.046 (3)
C8	1.293 (2)	0.1686 (9)	0.6277 (6)	0.040 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.0877 (7)	0.0859 (6)	0.0504 (5)	−0.0028 (6)	0.0114 (5)	0.0090 (4)
N	0.060 (7)	0.058 (5)	0.050 (5)	0.000 (5)	0.001 (5)	0.012 (4)
C1	0.085 (11)	0.051 (6)	0.070 (8)	−0.018 (7)	0.008 (8)	−0.007 (6)
C2	0.047 (7)	0.048 (6)	0.066 (7)	−0.017 (6)	0.000 (6)	−0.007 (5)
C3	0.034 (6)	0.039 (5)	0.050 (5)	0.007 (5)	−0.002 (5)	−0.004 (4)
C4	0.051 (7)	0.045 (5)	0.055 (6)	−0.006 (6)	−0.002 (6)	0.004 (5)
C5	0.052 (7)	0.041 (5)	0.043 (5)	0.003 (6)	0.001 (5)	0.002 (4)
C6	0.049 (8)	0.057 (6)	0.061 (7)	−0.005 (6)	0.004 (6)	0.013 (6)

C7	0.044 (6)	0.043 (5)	0.051 (6)	0.012 (6)	−0.019 (6)	−0.002 (5)
C8	0.028 (5)	0.047 (6)	0.045 (5)	0.002 (5)	0.001 (4)	−0.004 (4)

Geometric parameters (Å, °)

I—C5	2.101 (10)	N—H0A	0.8600
C1—C7	1.545 (16)	N—H0B	0.8600
C1—H1A	0.9600	C8—C3	1.372 (14)
C1—H1B	0.9600	C8—C7	1.421 (16)
C1—H1C	0.9600	C7—C6	1.389 (16)
C2—C3	1.537 (15)	C6—C5	1.380 (17)
C2—H2A	0.9600	C6—H6A	0.9300
C2—H2B	0.9600	C5—C4	1.359 (16)
C2—H2C	0.9600	C4—C3	1.373 (16)
N—C8	1.404 (14)	C4—H4A	0.9300
C7—C1—H1A	109.5	N—C8—C7	118.7 (9)
C7—C1—H1B	109.5	C6—C7—C8	118.4 (10)
H1A—C1—H1B	109.5	C6—C7—C1	121.3 (11)
C7—C1—H1C	109.5	C8—C7—C1	120.3 (10)
H1A—C1—H1C	109.5	C5—C6—C7	120.1 (11)
H1B—C1—H1C	109.5	C5—C6—H6A	120.0
C3—C2—H2A	109.5	C7—C6—H6A	120.0
C3—C2—H2B	109.5	C4—C5—C6	120.8 (10)
H2A—C2—H2B	109.5	C4—C5—I	121.7 (8)
C3—C2—H2C	109.5	C6—C5—I	117.5 (8)
H2A—C2—H2C	109.5	C5—C4—C3	120.5 (11)
H2B—C2—H2C	109.5	C5—C4—H4A	119.7
C8—N—H0A	120.0	C3—C4—H4A	119.7
C8—N—H0B	120.0	C8—C3—C4	120.4 (10)
H0A—N—H0B	120.0	C8—C3—C2	120.0 (10)
C3—C8—N	121.4 (10)	C4—C3—C2	119.6 (10)
C3—C8—C7	119.8 (10)		
C3—C8—C7—C6	−0.6 (16)	C6—C5—C4—C3	−0.7 (18)
N—C8—C7—C6	−176.2 (10)	I—C5—C4—C3	−179.5 (9)
C3—C8—C7—C1	178.8 (11)	N—C8—C3—C4	176.5 (11)
N—C8—C7—C1	3.2 (16)	C7—C8—C3—C4	1.1 (16)
C8—C7—C6—C5	−0.5 (17)	N—C8—C3—C2	−4.4 (16)
C1—C7—C6—C5	−179.9 (11)	C7—C8—C3—C2	−179.8 (10)
C7—C6—C5—C4	1.2 (18)	C5—C4—C3—C8	−0.5 (17)
C7—C6—C5—I	−180.0 (8)	C5—C4—C3—C2	−179.5 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0A···N^{i}	0.86	2.45	3.248 (12)	155

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1.

Fig. 1

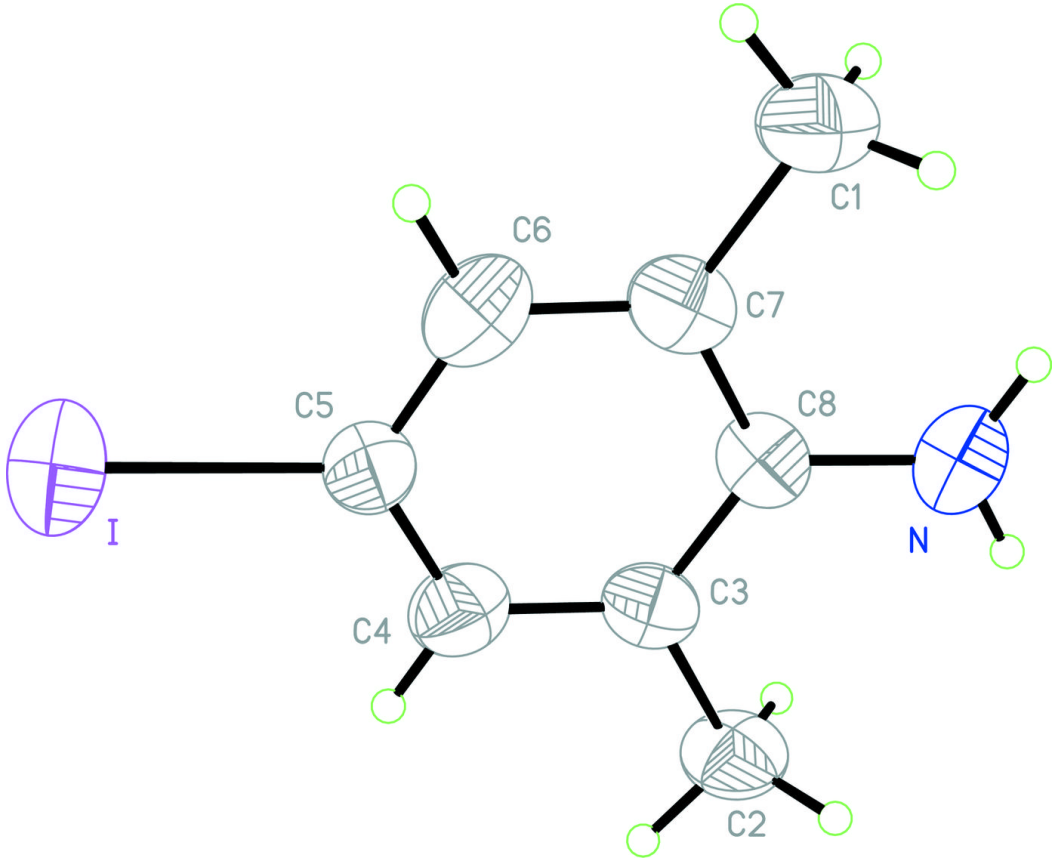

Fig. 2