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4-Iodo-2-methylaniline

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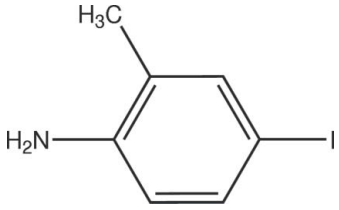
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.015 Å; R factor = 0.045; wR factor = 0.151; data-to-parameter ratio = 11.2.

In the molecule of the title compound, C_7H_8IN, the methyl C, I and N atoms lie in the benzene ring plane. In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules in a stacked arrangement along the *a* axis.

Related literature

For related literature, see: Kajigaeshi *et al.* (1988). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

C_7H_8IN
M_r = 233.04
Orthorhombic, $P2_12_12_1$
a = 5.5910 (11) Å
b = 8.9410 (18) Å
c = 15.674 (3) Å
V = 783.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.00 mm^{-1}
T = 294 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.487, T_{max} = 0.670
917 measured reflections
917 independent reflections
737 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.151
S = 1.04
917 reflections
82 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}
Absolute structure: Flack (1983), with no Friedel pairs
Flack parameter: −0.29 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0B···N^{i}	0.86	2.54	3.397 (15)	174

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

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: *PLATON-10M* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2418).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Kajigaeshi, S., Kakinami, T., Yamasaki, H., Fujisaki, S. & Okamoto, T. (1988). *Bull. Chem. Soc. Jpn*, **61**, 600–602.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

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S1. Comment

The title compound, (I), contains amino and halogen groups, which can react with different groups to prepare various function organic compounds. It is a kind of aromatic organic intermediate that can be used for many fields such as aromatic conductive polymer, organometallic chemistry *etc*. (Kajigaeshi *et al.*, 1988). We report herein its crystal structure.

In the molecule of (I), (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The atoms I, N and C7 lie in the benzene ring plane.

In the crystal structure, intermolecular N—H···N hydrogen bonds (Table 1) link the molecules stacked along the *a* axis, (Fig. 2), in which they may be effective in the stabilization of the structure.

S2. Experimental

The title compound, (I), was prepared by the literature method (Kajigaeshi *et al.*, 1988). Crystals suitable for X-ray analysis were obtained by dissolving (I) (0.5 g) in hexane (20 ml) and evaporating the solvent slowly at room temperature for about 7 d.

S3. 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.

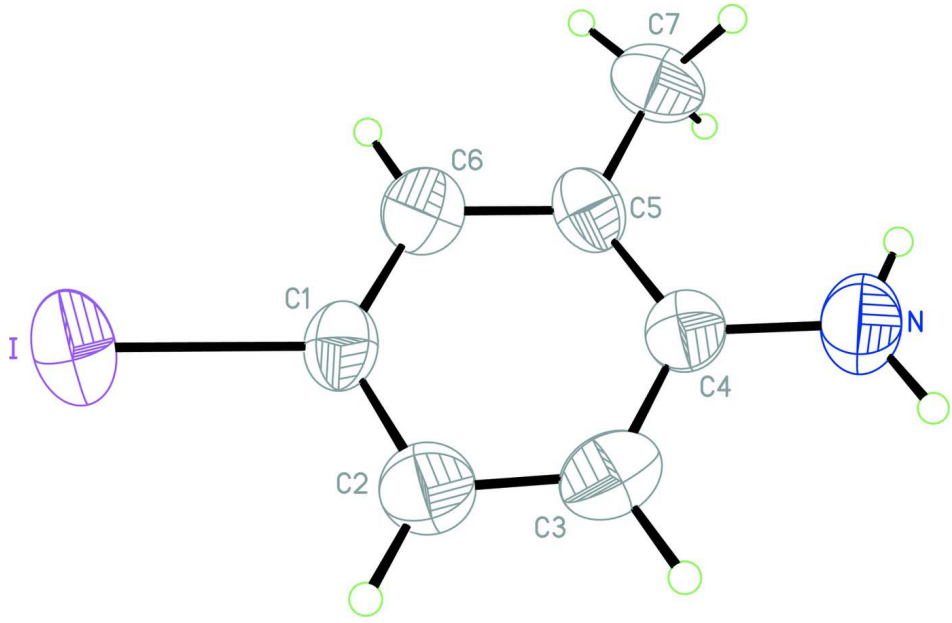

Figure 1

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

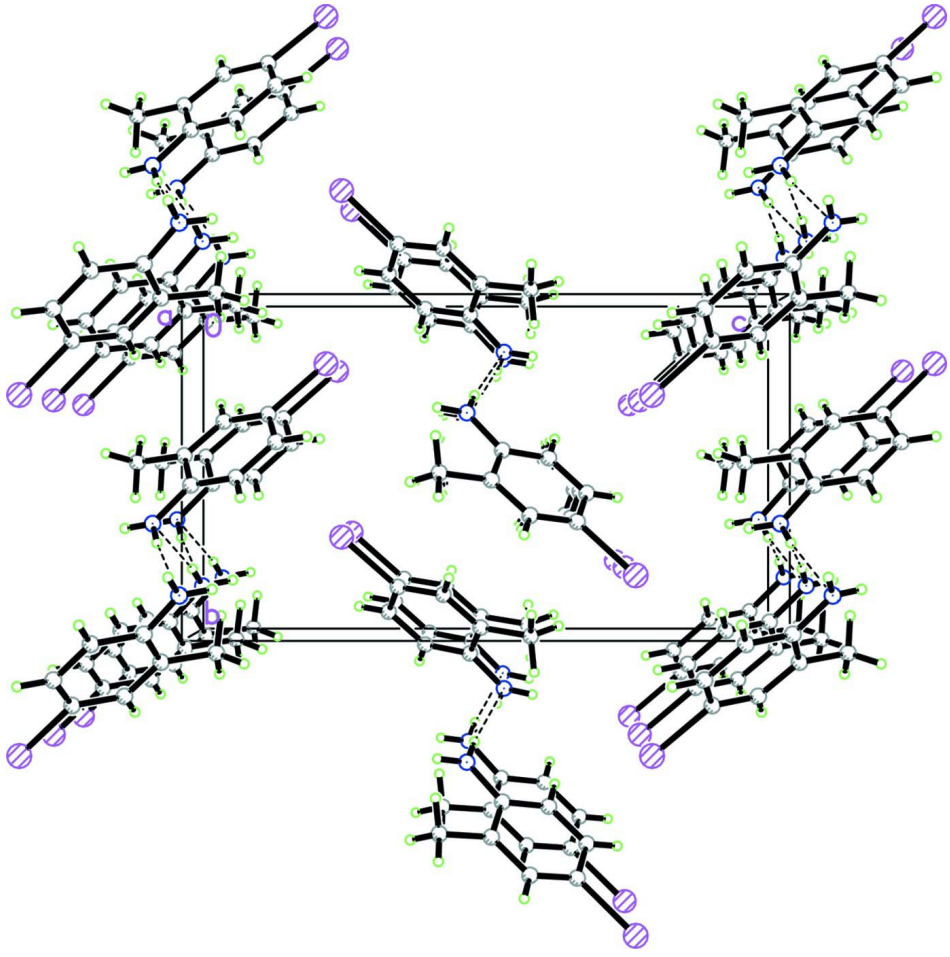

Figure 2

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

4-Iodo-2-methylaniline

Crystal data

C_7H_8IN
$M_r = 233.04$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.5910\ (11)$ Å
$b = 8.9410\ (18)$ Å
$c = 15.674\ (3)$ Å
$V = 783.5\ (3)$ Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.976$ Mg m^{-3}
Melting point: 360 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–$14°$
$\mu = 4.00$ mm^{-1}
$T = 294$ K
Block, purple
0.20 × 0.10 × 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)
$T_{min} = 0.487$, $T_{max} = 0.670$
917 measured reflections
917 independent reflections

737 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 19$
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.151$
$S = 1.04$
917 reflections
82 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 1.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}
Absolute structure: Flack (1983), with no Friedel pairs
Absolute structure parameter: −0.29 (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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I	0.01067 (18)	0.20097 (9)	0.23728 (5)	0.0696 (4)
N	0.407 (2)	0.6567 (10)	−0.0309 (8)	0.063 (3)
H0A	0.3335	0.6711	−0.0784	0.076*
H0B	0.5326	0.7081	−0.0188	0.076*
C1	0.1534 (18)	0.3484 (11)	0.1464 (7)	0.044 (2)
C2	0.360 (2)	0.4273 (12)	0.1643 (8)	0.053 (3)
H2A	0.4425	0.4137	0.2152	0.063*
C3	0.439 (2)	0.5276 (13)	0.1030 (7)	0.054 (3)
H3A	0.5772	0.5825	0.1139	0.064*
C4	0.322 (2)	0.5491 (11)	0.0269 (7)	0.042 (2)
C5	0.122 (2)	0.4658 (11)	0.0088 (7)	0.045 (2)
C6	0.028 (2)	0.3671 (11)	0.0701 (7)	0.051 (3)
H6A	−0.1143	0.3158	0.0601	0.062*
C7	−0.011 (2)	0.4852 (13)	−0.0736 (7)	0.059 (3)
H7A	−0.1480	0.4207	−0.0741	0.089*
H7B	0.0924	0.4599	−0.1204	0.089*
H7C	−0.0615	0.5873	−0.0791	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.0908 (7)	0.0662 (5)	0.0517 (5)	−0.0067 (5)	0.0050 (5)	0.0104 (3)
N	0.061 (6)	0.051 (5)	0.078 (7)	−0.004 (5)	0.007 (6)	0.012 (5)
C1	0.048 (6)	0.044 (5)	0.038 (5)	0.002 (5)	0.011 (5)	−0.001 (4)
C2	0.056 (7)	0.052 (6)	0.050 (6)	−0.005 (5)	−0.005 (6)	−0.005 (5)
C3	0.041 (6)	0.055 (7)	0.064 (7)	−0.001 (5)	0.001 (5)	−0.010 (6)
C4	0.040 (6)	0.043 (6)	0.043 (5)	0.006 (4)	0.009 (5)	−0.002 (4)
C5	0.058 (7)	0.036 (5)	0.040 (5)	0.005 (5)	0.002 (5)	0.001 (4)
C6	0.056 (7)	0.044 (5)	0.054 (6)	−0.005 (6)	−0.001 (6)	−0.006 (4)
C7	0.063 (7)	0.065 (6)	0.050 (5)	0.013 (9)	−0.009 (8)	−0.006 (5)

Geometric parameters (Å, º)

I—C1	2.099 (10)	C4—C5	1.374 (16)
N—H0A	0.8600	C4—N	1.403 (13)
N—H0B	0.8600	C5—C6	1.408 (15)
C1—C2	1.383 (15)	C6—H6A	0.9300
C1—C6	1.397 (15)	C7—C5	1.500 (15)
C2—C3	1.386 (16)	C7—H7A	0.9600
C2—H2A	0.9300	C7—H7B	0.9600
C3—C4	1.375 (16)	C7—H7C	0.9600
C3—H3A	0.9300		
C4—N—H0A	120.0	C3—C4—N	119.7 (11)
C4—N—H0B	120.0	C4—C5—C6	120.3 (10)
H0A—N—H0B	120.0	C4—C5—C7	121.2 (10)
C2—C1—C6	122.2 (10)	C6—C5—C7	118.3 (11)
C2—C1—I	120.0 (8)	C1—C6—C5	118.1 (10)
C6—C1—I	117.7 (8)	C1—C6—H6A	121.0
C1—C2—C3	117.2 (10)	C5—C6—H6A	121.0
C1—C2—H2A	121.4	C5—C7—H7A	109.5
C3—C2—H2A	121.4	C5—C7—H7B	109.5
C4—C3—C2	122.7 (10)	H7A—C7—H7B	109.5
C4—C3—H3A	118.6	C5—C7—H7C	109.5
C2—C3—H3A	118.6	H7A—C7—H7C	109.5
C5—C4—C3	119.4 (10)	H7B—C7—H7C	109.5
C5—C4—N	120.9 (11)		
C6—C1—C2—C3	0.2 (16)	C3—C4—C5—C6	4.6 (16)
I—C1—C2—C3	−177.3 (8)	N—C4—C5—C6	−174.8 (9)
C2—C1—C6—C5	2.5 (16)	C3—C4—C5—C7	−179.8 (10)
I—C1—C6—C5	180.0 (7)	N—C4—C5—C7	0.8 (15)
C1—C2—C3—C4	−0.5 (17)	C4—C5—C6—C1	−4.9 (16)
C2—C3—C4—C5	−1.8 (17)	C7—C5—C6—C1	179.4 (10)
C2—C3—C4—N	177.5 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0*B*···N^{i}	0.86	2.54	3.397 (15)	174

Symmetry code: (i) *x*+1/2, −*y*+3/2, −*z*.