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2-Iodo-4,6-dimethylpyrimidine

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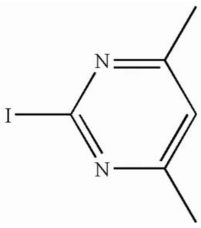
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 14.3.

In the title compound, $C_6H_7IN_2$, the non-H atoms of the molecule are located on a crystallographic mirror plane; the H atoms of the methyl groups are therefore disordered over two positions of equal occupancy. In the crystal structure, short intermolecular I$\cdots$N contacts [3.390 (3) Å] are found, linking the molecules into zigzag chains. In addition, there are intermolecular π–π stacking interactions between the pyrimidine rings of adjacent molecules [centroid–centroid distance = 3.5168 (10) Å], resulting in a two-dimensional supramolecular architecture.

Related literature

For applications of pyrimidine derivatives, see: Chinchilla *et al.* (2004); Xu *et al.* (2009*a*,*b*). For halogen–electronegative atom interactions, see: Lommerse *et al.* (1996). For the synthesis of 4,6-dimethyl-2-chloropyrimidine, see: Kosolapoff & Roy (1961) and literature cited therein.



Experimental

Crystal data

$C_6H_7IN_2$
M_r = 234.04
Orthorhombic, *Pnma*
a = 7.930 (2) Å
b = 7.0256 (19) Å
c = 14.499 (4) Å
V = 807.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.88 mm^{-1}
T = 296 K
0.32 × 0.25 × 0.21 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.370, $T_{\max}$ = 0.496
5541 measured reflections
817 independent reflections
739 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.066
S = 1.10
817 reflections
57 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.81 e Å^{-3}
$\Delta\rho_{\min}$ = −0.21 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2242).

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supplementary materials

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2-Iodo-4,6-dimethylpyrimidine

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Comment

Some derivatives of pyrimidine are important chemical materials (Chinchilla *et al.*, 2004). Among them, 4,6-dimethyl-2-iodopyrimidine is a good partner in cross-coupling reaction giving a variety of pyrimidine ligands (Xu *et al.*, 2009a, b). The molecular structure of the related title compound is shown in Fig. 1. The molecule is located on a crystallographic mirror plane, thus the H atoms of the methyl groups are disordered over two positions, with site-occupation factors fixed at 0.5. The interesting feature of the crystal structure is short intermolecular I···N contacts [3.390 (3) Å] (Lommerse *et al.*, 1996), which is obviously shorter than the sum of the van der Waals radii of the relevant atoms. In addtion, there are strong intermolecular π—π stacking interactions between the pyrimidine rings of adjacent molecules [centroid-centroid distance = 3.5168 (10) Å], resulting in a two-dimensional supramolecular architecture (Fig.2).

Experimental

The title compound was prepared as described in literature (Kosolapoff & Roy 1961) and recrystallized from dichloromethane-petroleum ether solution at room temperature to give the desired product as colourless crystals suitable for single-crystal X-ray diffraction.

Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) and (1.5$U_{\rm eq}$ for methyl H).

Figures

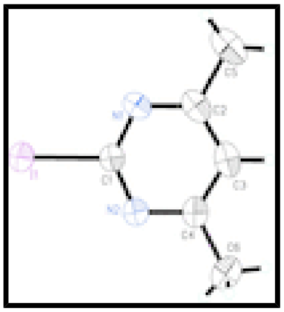

Fig. 1. The molecular structure of the title compound with displacement ellipsoids at the 30% probability level, the disordered H atoms are omitted.

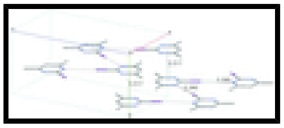

Fig. 2. Partial view of the crystal packing showing the short intermolecular I···N contacts and π—π stacking interactions.

2-Iodo-4,6-dimethylpyrimidine

Crystal data

$C_6H_7IN_2$	$D_x = 1.924$ Mg m^{-3}
$M_r = 234.04$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pnma*	Cell parameters from 2976 reflections
$a = 7.930$ (2) Å	$\theta = 2.8$–$24.9°$
$b = 7.0256$ (19) Å	$\mu = 3.88$ mm^{-1}
$c = 14.499$ (4) Å	$T = 296$ K
$V = 807.8$ (4) Å^3	Block, colourless
$Z = 4$	$0.32 \times 0.25 \times 0.21$ mm
$F(000) = 440$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	817 independent reflections
Radiation source: fine-focus sealed tube	739 reflections with $I > 2\sigma(I)$
graphite	$R_{\text{int}} = 0.029$
phi and ω scans	$\theta_{\text{max}} = 25.5°$, $\theta_{\text{min}} = 2.8°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.370$, $T_{\text{max}} = 0.496$	$k = -8 \rightarrow 8$
5541 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.066$	H-atom parameters constrained
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.259P]$ where $P = (F_o^2 + 2F_c^2)/3$
817 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
57 parameters	$\Delta\rho_{\text{max}} = 0.81$ e Å^{-3}
0 restraints	$\Delta\rho_{\text{min}} = -0.21$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}	Occ. (<1)
C1	0.4205 (6)	0.2500	0.4216 (3)	0.0559 (10)	
C2	0.4224 (8)	0.2500	0.5763 (3)	0.0708 (13)	
C3	0.5963 (8)	0.2500	0.5741 (3)	0.0746 (14)	
H3	0.6587	0.2500	0.6285	0.090*	
C4	0.6751 (7)	0.2500	0.4899 (3)	0.0680 (12)	
C5	0.3278 (11)	0.2500	0.6665 (5)	0.108 (2)	
H5A	0.2299	0.1703	0.6612	0.162*	0.50
H5B	0.2935	0.3775	0.6812	0.162*	0.50
H5C	0.3996	0.2022	0.7145	0.162*	0.50
C6	0.8651 (8)	0.2500	0.4820 (5)	0.107 (2)	
H6A	0.9047	0.1215	0.4761	0.161*	0.50
H6B	0.9132	0.3068	0.5361	0.161*	0.50
H6C	0.8980	0.3218	0.4286	0.161*	0.50
I1	0.27885 (5)	0.2500	0.29859 (2)	0.07396 (18)	
N1	0.3314 (6)	0.2500	0.4980 (2)	0.0656 (9)	
N2	0.5862 (5)	0.2500	0.4101 (2)	0.0616 (9)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.063 (3)	0.046 (2)	0.058 (2)	0.000	−0.002 (2)	0.000
C2	0.107 (4)	0.047 (2)	0.058 (3)	0.000	0.007 (3)	0.000
C3	0.106 (4)	0.059 (3)	0.059 (3)	0.000	−0.014 (3)	0.000
C4	0.076 (3)	0.064 (3)	0.064 (3)	0.000	−0.012 (2)	0.000
C5	0.158 (7)	0.098 (4)	0.068 (3)	0.000	0.022 (4)	0.000
C6	0.073 (4)	0.151 (6)	0.098 (4)	0.000	−0.014 (3)	0.000
I1	0.0685 (3)	0.0874 (3)	0.0660 (3)	0.000	−0.01043 (13)	0.000

N1	0.075 (2)	0.065 (2)	0.057 (2)	0.000	0.0106 (19)	0.000
N2	0.064 (2)	0.062 (2)	0.059 (2)	0.000	−0.0017 (17)	0.000

Geometric parameters (Å, °)

C1—N1	1.314 (6)	C4—N2	1.356 (6)
C1—N2	1.325 (6)	C4—C6	1.511 (9)
C1—I1	2.108 (4)	C5—H5A	0.9600
C2—N1	1.345 (7)	C5—H5B	0.9600
C2—C3	1.380 (9)	C5—H5C	0.9600
C2—C5	1.507 (8)	C6—H6A	0.9600
C3—C4	1.371 (7)	C6—H6B	0.9600
C3—H3	0.9300	C6—H6C	0.9600
N1—C1—N2	129.8 (4)	C2—C5—H5B	109.5
N1—C1—I1	115.3 (3)	H5A—C5—H5B	109.5
N2—C1—I1	114.9 (3)	C2—C5—H5C	109.5
N1—C2—C3	121.1 (5)	H5A—C5—H5C	109.5
N1—C2—C5	117.7 (6)	H5B—C5—H5C	109.5
C3—C2—C5	121.2 (6)	C4—C6—H6A	109.5
C4—C3—C2	118.4 (5)	C4—C6—H6B	109.5
C4—C3—H3	120.8	H6A—C6—H6B	109.5
C2—C3—H3	120.8	C4—C6—H6C	109.5
N2—C4—C3	121.6 (5)	H6A—C6—H6C	109.5
N2—C4—C6	116.9 (4)	H6B—C6—H6C	109.5
C3—C4—C6	121.5 (5)	C1—N1—C2	115.1 (5)
C2—C5—H5A	109.5	C1—N2—C4	114.1 (4)
N1—C2—C3—C4	0.0	C3—C2—N1—C1	0.0
C5—C2—C3—C4	180.0	C5—C2—N1—C1	180.0
C2—C3—C4—N2	0.0	N1—C1—N2—C4	0.0
C2—C3—C4—C6	180.0	I1—C1—N2—C4	180.0
N2—C1—N1—C2	0.0	C3—C4—N2—C1	0.00
I1—C1—N1—C2	180.0	C6—C4—N2—C1	180.0

Fig. 1

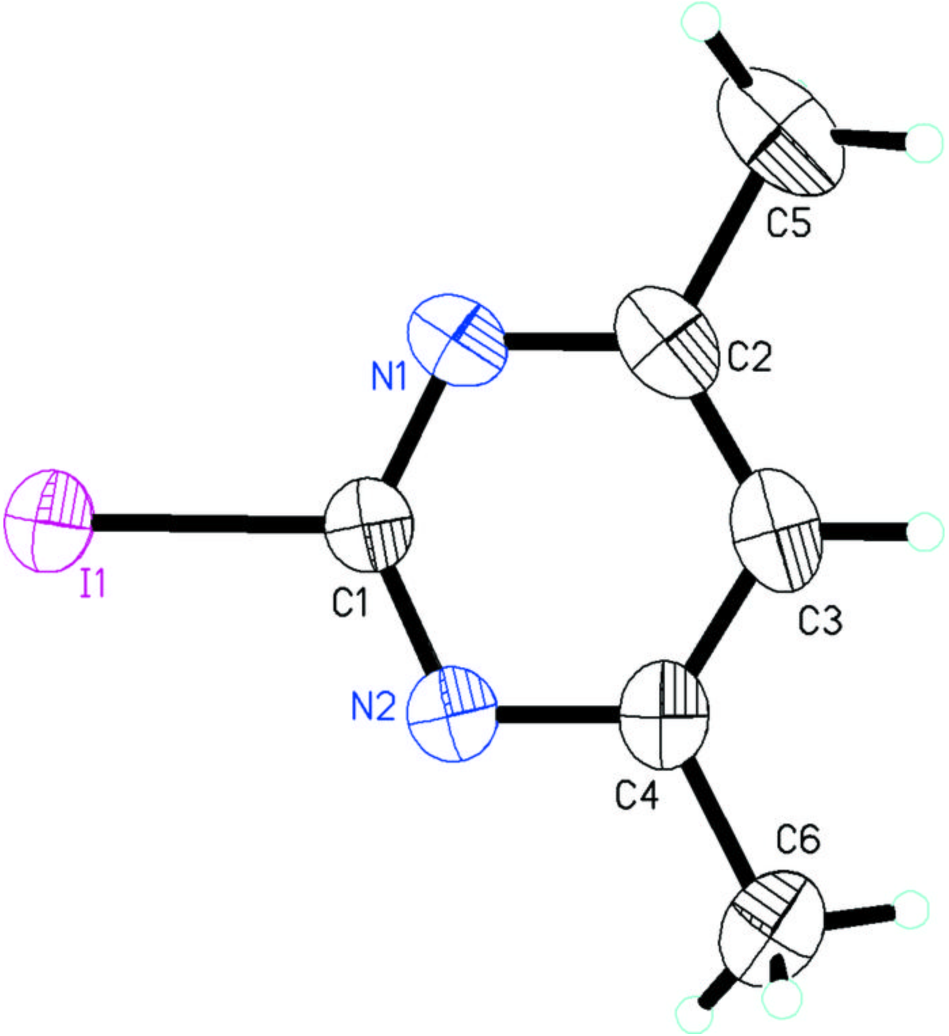

Fig. 2