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## Structure Reports

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4,6-Dimethyl-2-*p*-tolylpyrimidineChen Xu,<sup>a\*</sup> Zhi-Qiang Wang,<sup>a</sup> Fei-Fei Cen,<sup>b</sup> Lin Cheng<sup>b</sup> and Bao-Ming Ji<sup>a</sup><sup>a</sup>College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, People's Republic of China, and <sup>b</sup>Chemical Engineering and Pharmaceutics School, Henan University of Science and Technology, Luoyang 471003, People's Republic of China

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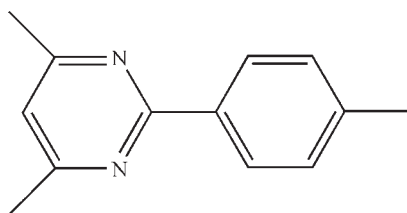
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.131; data-to-parameter ratio = 14.0.

The molecule of the title compound,  $\text{C}_{13}\text{H}_{14}\text{N}_2$ , is located on a crystallographic mirror plane. The aromatic rings make a dihedral angle of  $3.4(2)^\circ$ . The H atoms of the methyl groups on the benzene ring are disordered over two positions; their site-occupation factors were fixed at 0.5. In the crystal, intermolecular  $\text{C}-\text{H}\cdots\pi$  contacts form infinite chains perpendicular to the  $b$  axis.

## Related literature

The title compound was derived from the reaction of *p*-tolylmercuric chlorides and 4,6-dimethyl-2-iodopyrimidine. For general background to these of organomercury compounds in cross-coupling reactions, see: Beletskaya *et al.* (2001); Braga *et al.* (2004). For a related structure, see: Santoni *et al.* (2008). For the synthesis, see: Xu *et al.* (2009a,b).



## Experimental

## Crystal data

 $\text{C}_{13}\text{H}_{14}\text{N}_2$  $M_r = 198.26$ Orthorhombic,  $Pnma$  $a = 7.2086(10)$  Å $b = 12.4668(18)$  Å $c = 12.4335(18)$  Å $V = 1117.4(3)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.07$  mm<sup>-1</sup> $T = 296$  K $0.35 \times 0.25 \times 0.22$  mm

## Data collection

Bruker SMART APEX CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.976$ ,  $T_{\max} = 0.985$ 

7934 measured reflections

1089 independent reflections

777 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.025$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$  $wR(F^2) = 0.131$  $S = 1.06$ 

1089 reflections

78 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.14$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8}\cdots\text{Cg1}^i$	0.93	2.79	3.638 (2)	152

Symmetry code: (i)  $-x - 1, y + \frac{1}{2}, -z$ . Cg1 is the centroid of the pyrimidine ring.

Data collection: SMART (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 and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2211).

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**supplementary materials**

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## 4,6-Dimethyl-2-*p*-tolylpyrimidine

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### Comment

The organomercury compounds have a number of notable advantages over other organometallic compounds commonly used in cross-coupling reactions, including higher selectivity of reactions, extra stability and easy availability by a direct mercuration (Beletskaya *et al.*, 2001; Braga *et al.*, 2004). We have recently reported ferrocene-heterocycles were obtained from the coupling reaction (Xu *et al.*, 2009a,b). Here we report the crystal structure of the title compound, derived from the reaction of *p*-tolylmercuric chlorides and 4,6-dimethyl-2-iodopyrimidine.

Due to the molecular mirror symmetry *m* of the title compound (Fig.1), and coincidence with the crystallographic mirror plane *m* (space group *Pnma*), the atoms C1, C2, C5, C8, H8 are half occupied and the H atoms of the methyl groups in the benzene ring are disordered over two positions; their site-occupation factors were fixed at 0.5. The aromatic rings have very small angles between their planes (dihedral angle is 3.4 (2)°) due to the absence of H—H repulsion (Santoni *et al.*, 2008). Fig.2 shows that in the crystal there exist intermolecular C—H··· $\pi$  interactions (Table 1, Cg1 is the centroid of the pyrimidine ring).

### Experimental

The title compound was obtained from the coupling reaction of *p*-tolylmercuric chlorides and 4,6-dimethyl-2-iodopyrimidine as described in literature (Xu *et al.*, 2009b) and recrystallized from ethanol at room temperature to give the desired 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  $U_{\text{iso}}(\text{H})=1.2\text{--}1.5U_{\text{eq}}(\text{C})$ .

### Figures

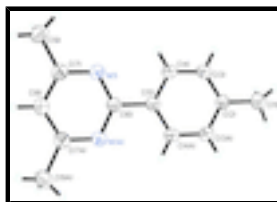


Fig. 1. The molecular structure of the title compound with displacement ellipsoids at the 30% probability level, the disordered H atoms are omitted (Symmetry code A:  $-x + 2, -y, -z$ ).

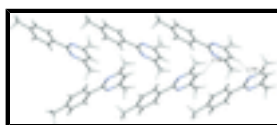


Fig. 2. Partial view of the crystal packing showing the formation of the infinite chain of molecules formed by the C—H··· $\pi$  interactions.

## 4,6-Dimethyl-2-*p*-tolylpyrimidine

### Crystal data

$C_{13}H_{14}N_2$	$D_x = 1.179 \text{ Mg m}^{-3}$
$M_r = 198.26$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $Pnma$	Cell parameters from 1634 reflections
$a = 7.2086 (10) \text{ \AA}$	$\theta = 2.3\text{--}23.3^\circ$
$b = 12.4668 (18) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$c = 12.4335 (18) \text{ \AA}$	$T = 296 \text{ K}$
$V = 1117.4 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.35 \times 0.25 \times 0.22 \text{ mm}$
$F_{000} = 424$	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	1089 independent reflections
Radiation source: fine-focus sealed tube	777 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.025$
$T = 296 \text{ K}$	$\theta_{\text{max}} = 25.5^\circ$
phi and $\omega$ scans	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\text{min}} = 0.976$ , $T_{\text{max}} = 0.985$	$k = -15 \rightarrow 15$
7934 measured reflections	$l = -15 \rightarrow 14$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.291P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
1089 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
78 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
	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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.8988 (4)	0.2500	0.6728 (2)	0.0709 (8)	
H1A	0.8781	0.2870	0.7394	0.106*	0.50
H1B	0.9952	0.2856	0.6332	0.106*	0.50
H1C	0.9355	0.1774	0.6874	0.106*	0.50
C2	0.7231 (3)	0.2500	0.60770 (17)	0.0499 (6)	
C3	0.6383 (2)	0.34507 (13)	0.57708 (13)	0.0544 (5)	
H3	0.6934	0.4100	0.5953	0.065*	
C4	0.4741 (2)	0.34546 (12)	0.52012 (13)	0.0522 (5)	
H4	0.4201	0.4105	0.5009	0.063*	
C5	0.3884 (3)	0.2500	0.49107 (16)	0.0449 (5)	
C6	0.2078 (3)	0.2500	0.43367 (17)	0.0468 (5)	
C7	-0.0325 (2)	0.34504 (13)	0.36089 (13)	0.0529 (5)	
C8	-0.1188 (3)	0.2500	0.33466 (18)	0.0549 (6)	
H8	-0.2331	0.2500	0.3000	0.066*	
C9	-0.1170 (3)	0.45227 (14)	0.33570 (16)	0.0732 (6)	
H9A	-0.0974	0.5001	0.3951	0.110*	
H9B	-0.2477	0.4438	0.3235	0.110*	
H9C	-0.0598	0.4814	0.2724	0.110*	
N1	0.13292 (18)	0.34589 (10)	0.41062 (10)	0.0509 (4)	

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0703 (17)	0.0703 (18)	0.0720 (17)	0.000	-0.0169 (14)	0.000
C2	0.0541 (14)	0.0531 (13)	0.0425 (11)	0.000	-0.0007 (10)	0.000

## supplementary materials

C3	0.0600 (11)	0.0446 (9)	0.0584 (10)	-0.0043 (8)	-0.0036 (8)	-0.0048 (7)
C4	0.0588 (10)	0.0390 (9)	0.0589 (10)	0.0022 (7)	-0.0028 (8)	0.0002 (7)
C5	0.0507 (12)	0.0407 (11)	0.0433 (11)	0.000	0.0027 (10)	0.000
C6	0.0545 (13)	0.0430 (12)	0.0428 (11)	0.000	0.0018 (10)	0.000
C7	0.0550 (10)	0.0541 (10)	0.0496 (9)	0.0045 (8)	0.0009 (7)	0.0034 (7)
C8	0.0510 (13)	0.0608 (15)	0.0528 (13)	0.000	-0.0047 (11)	0.000
C9	0.0702 (12)	0.0598 (12)	0.0896 (14)	0.0091 (10)	-0.0128 (10)	0.0094 (10)
N1	0.0546 (8)	0.0449 (8)	0.0532 (8)	0.0031 (6)	-0.0025 (6)	0.0021 (6)

### Geometric parameters (Å, °)

C1—C2	1.503 (3)	C5—C6	1.485 (3)
C1—H1A	0.9600	C6—N1 <sup>i</sup>	1.3426 (16)
C1—H1B	0.9600	C6—N1	1.3426 (16)
C1—H1C	0.9600	C7—N1	1.343 (2)
C2—C3 <sup>i</sup>	1.387 (2)	C7—C8	1.378 (2)
C2—C3	1.387 (2)	C7—C9	1.502 (2)
C3—C4	1.380 (2)	C8—C7 <sup>i</sup>	1.378 (2)
C3—H3	0.9300	C8—H8	0.9300
C4—C5	1.3885 (19)	C9—H9A	0.9600
C4—H4	0.9300	C9—H9B	0.9600
C5—C4 <sup>i</sup>	1.3885 (19)	C9—H9C	0.9600
C2—C1—H1A	109.5	C4 <sup>i</sup> —C5—C6	121.00 (11)
C2—C1—H1B	109.5	N1 <sup>i</sup> —C6—N1	125.8 (2)
H1A—C1—H1B	109.5	N1 <sup>i</sup> —C6—C5	117.07 (10)
C2—C1—H1C	109.5	N1—C6—C5	117.07 (10)
H1A—C1—H1C	109.5	N1—C7—C8	121.12 (16)
H1B—C1—H1C	109.5	N1—C7—C9	116.67 (15)
C3 <sup>i</sup> —C2—C3	117.4 (2)	C8—C7—C9	122.20 (16)
C3 <sup>i</sup> —C2—C1	121.28 (11)	C7—C8—C7 <sup>i</sup>	118.7 (2)
C3—C2—C1	121.28 (11)	C7—C8—H8	120.7
C4—C3—C2	121.48 (16)	C7 <sup>i</sup> —C8—H8	120.7
C4—C3—H3	119.3	C7—C9—H9A	109.5
C2—C3—H3	119.3	C7—C9—H9B	109.5
C3—C4—C5	120.81 (16)	H9A—C9—H9B	109.5
C3—C4—H4	119.6	C7—C9—H9C	109.5
C5—C4—H4	119.6	H9A—C9—H9C	109.5
C4—C5—C4 <sup>i</sup>	118.0 (2)	H9B—C9—H9C	109.5
C4—C5—C6	121.00 (11)	C6—N1—C7	116.62 (15)
C3 <sup>i</sup> —C2—C3—C4	1.2 (3)	C4 <sup>i</sup> —C5—C6—N1	178.65 (17)
C1—C2—C3—C4	-178.02 (19)	N1—C7—C8—C7 <sup>i</sup>	0.3 (3)
C2—C3—C4—C5	-0.3 (3)	C9—C7—C8—C7 <sup>i</sup>	-179.77 (14)
C3—C4—C5—C4 <sup>i</sup>	-0.7 (3)	N1 <sup>i</sup> —C6—N1—C7	0.6 (3)
C3—C4—C5—C6	177.47 (16)	C5—C6—N1—C7	-178.53 (15)
C4—C5—C6—N1 <sup>i</sup>	-178.65 (17)	C8—C7—N1—C6	-0.4 (3)

C4 <sup>i</sup> —C5—C6—N1 <sup>i</sup>	-0.6 (3)	C9—C7—N1—C6	179.62 (16)
C4—C5—C6—N1	0.6 (3)		

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

*Hydrogen-bond geometry* (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8···Cg1 <sup>ii</sup>	0.93	2.79	3.638 (2)	152

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

Fig. 1

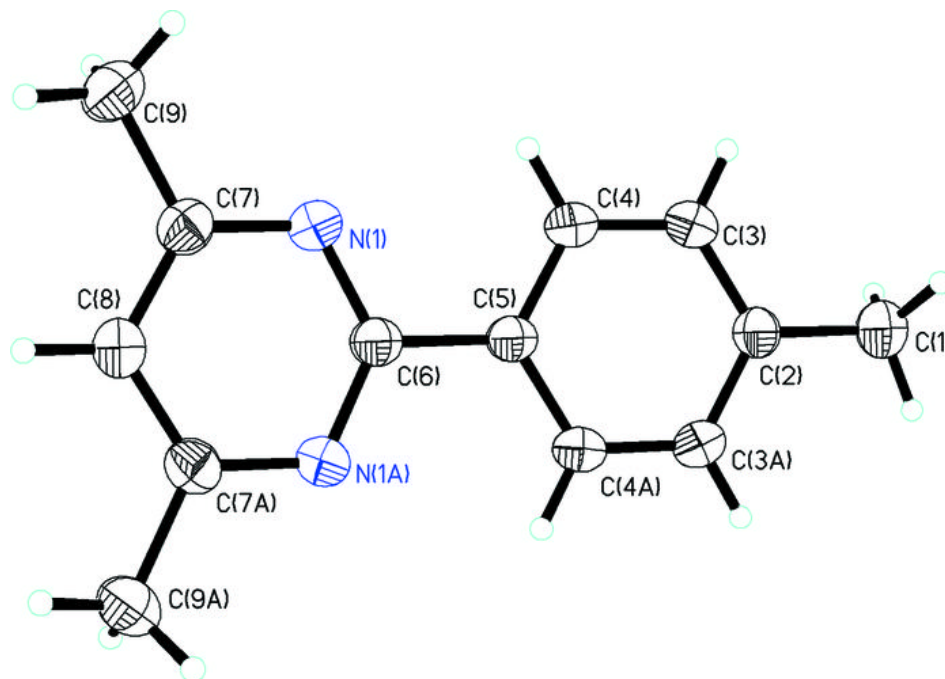




Fig. 2

