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## Structure Reports

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## 2-Chloro-*N*-(2,4-dimethylphenyl)-acetamide

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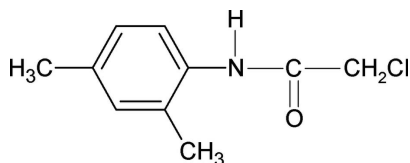
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 Key indicators: single-crystal X-ray study;  $T = 299$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.067;  $wR$  factor = 0.190; data-to-parameter ratio = 14.8.

The conformation of the N—H bond in the structure of the title compound,  $\text{C}_{10}\text{H}_{12}\text{ClNO}$ , is *syn* to the *ortho* methyl group, similar to that observed with respect to the *meta* methyl group in 2-chloro-*N*-(3-methylphenyl)acetamide and the *ortho*-chloro group in 2-chloro-*N*-(2-chlorophenyl)acetamide. The geometric parameters are similar to those of other acetanilides. The molecules are linked into chains through intermolecular N—H $\cdots$ O hydrogen bonds.

### Related literature

For related literature, see: Gowda *et al.* (2007*a,b,c,d,e,f*, 2008); Shilpa & Gowda (2007).



### Experimental

#### Crystal data

 $\text{C}_{10}\text{H}_{12}\text{ClNO}$ 
 $M_r = 197.66$ 

 Triclinic,  $P\bar{1}$ 
 $a = 4.7235$  (7) Å

 $b = 10.407$  (2) Å

 $c = 11.451$  (2) Å

 $\alpha = 67.07$  (2)°

 $\beta = 86.84$  (1)°

 $\gamma = 78.95$  (2)°

 $V = 508.69$  (15) Å<sup>3</sup>
 $Z = 2$ 

 Cu  $K\alpha$  radiation

 $\mu = 3.00$  mm<sup>-1</sup>
 $T = 299$  (2) K

 $0.60 \times 0.06 \times 0.04$  mm

#### Data collection

Enraf–Nonius CAD-4

diffractometer

 Absorption correction:  $\psi$  scan

 (North *et al.*, 1968)

 $T_{\min} = 0.803$ ,  $T_{\max} = 0.895$ 

2059 measured reflections

1817 independent reflections

 1394 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.015$ 

3 standard reflections

frequency: 120 min

intensity decay: 1.0%

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.067$ 
 $wR(F^2) = 0.190$ 
 $S = 1.09$ 

1817 reflections

123 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.45$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.47$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}^i$	0.83 (4)	2.04 (4)	2.853 (3)	165 (3)

 Symmetry code: (i)  $x + 1, y, z$ .

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2650).

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## supporting information

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### 2-Chloro-*N*-(2,4-dimethylphenyl)acetamide

**B. Thimme Gowda, Sabine Foro and Hartmut Fuess**

#### S1. Comment

In the present work, the structure of 2-chloro-*N*-(2,4-dimethylphenyl)- acetamide (24DMPCA) has been determined as part of a study of the effect of ring and side chain substitutions on the solid state geometry of aromatic amides (Gowda *et al.*, 2007*a, b, c, d, e*). The conformation of the N—H bond in the structure of 24DMPCA is *syn* to the *ortho* methyl group (Fig. 1), similar to that observed with respect to the *meta* methyl group in the 2-chloro- *N*-(3-methylphenyl)acetamide (3MPCA)(Gowda *et al.*, 2007*e*). and *ortho* chloro group in the 2-chloro-*N*-(2-chlorophenyl)- acetamide(2CPCA)(Gowda *et al.*, 2007*d*). The geometric parameters in 24DMPCA are similar to those in 3MPCA (Gowda *et al.*, 2007*e*), 2CPCA (Gowda *et al.*, 2007*d*), 2-chloro-*N*-(4-methylphenyl)- acetamide (Gowda *et al.*, 2007*b*), 2-chloro-*N*- (4-chlorophenyl)- acetamide (Gowda *et al.*, 2007*c*) and other acetanilides (Gowda *et al.* , 2007*a*). The molecules in the structure are linked into chains through intermolecular N—H···O hydrogen bonding (Table 1 and Fig.2).

#### S2. Experimental

The title compound was prepared according to the literature method (Shilpa and Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Shilpa and Gowda, 2007). Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

#### S3. Refinement

The CH atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.97 Å. The NH atom was located in difference map and its coordinates were refined.  $U_{\text{iso}}(\text{H})$  values were set equal to 1.2  $U_{\text{eq}}(\text{C}, \text{N})$  or 1.2  $U_{\text{eq}}(\text{C}_{\text{methyl}})$ .

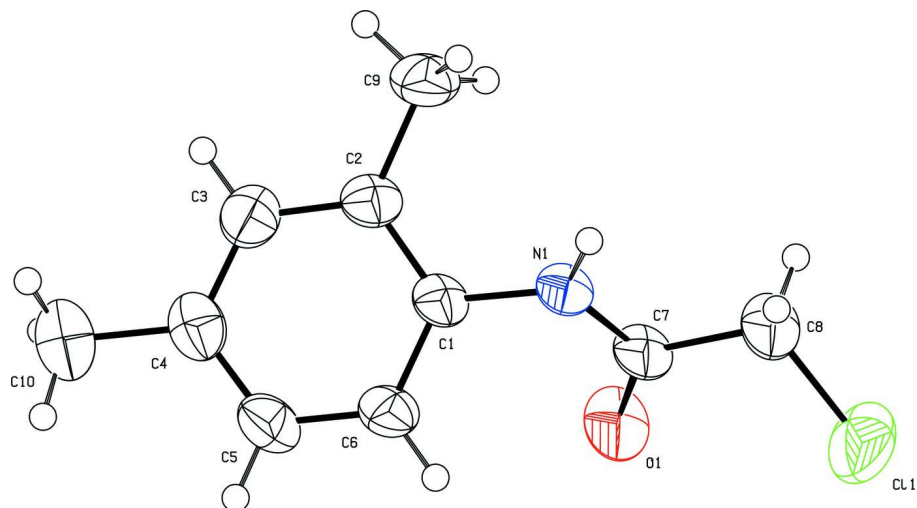


Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

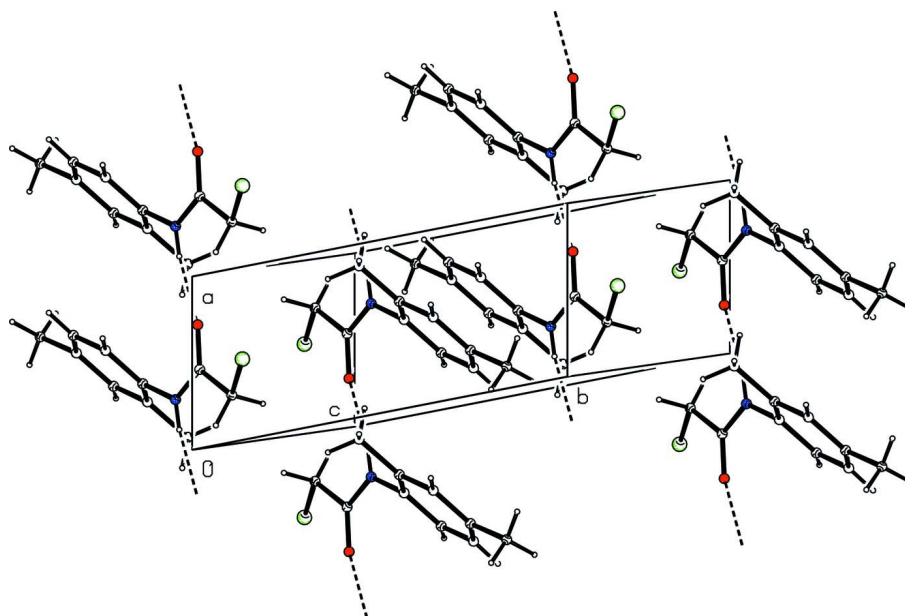


Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

### 2-Chloro-*N*-(2,4-dimethylphenyl)acetamide

#### Crystal data

$C_{10}H_{12}ClNO$

$M_r = 197.66$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 4.7235\ (7)\ \text{\AA}$

$b = 10.407\ (2)\ \text{\AA}$

$c = 11.451\ (2)\ \text{\AA}$

$\alpha = 67.07\ (2)^\circ$

$\beta = 86.84\ (1)^\circ$

$\gamma = 78.95\ (2)^\circ$

$V = 508.69\ (15)\ \text{\AA}^3$

$Z = 2$

$F(000) = 208$

$D_x = 1.290\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54180 \text{ \AA}$   
 Cell parameters from 25 reflections  
 $\theta = 4.2\text{--}26.4^\circ$   
 $\mu = 3.00 \text{ mm}^{-1}$

$T = 299 \text{ K}$   
 Needle, colourless  
 $0.60 \times 0.06 \times 0.04 \text{ mm}$

*Data collection*

Enraf–Nonius CAD-4  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan  
 North *et al.* (1968)  
 $T_{\min} = 0.803$ ,  $T_{\max} = 0.895$   
 2059 measured reflections

1817 independent reflections  
 1394 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.015$   
 $\theta_{\max} = 66.9^\circ$ ,  $\theta_{\min} = 4.2^\circ$   
 $h = 0 \rightarrow 5$   
 $k = -12 \rightarrow 12$   
 $l = -13 \rightarrow 13$   
 3 standard reflections every 120 min  
 intensity decay: 1.0%

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.067$   
 $wR(F^2) = 0.190$   
 $S = 1.09$   
 1817 reflections  
 123 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 atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.1035P)^2 + 0.2646P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.044$   
 $\Delta\rho_{\max} = 0.45 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.47 \text{ e \AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.5208 (2)	−0.02640 (14)	0.75189 (11)	0.1062 (6)
O1	0.2611 (4)	0.1946 (3)	0.5165 (2)	0.0695 (8)
N1	0.6642 (5)	0.2847 (3)	0.4451 (2)	0.0411 (6)
H1N	0.842 (8)	0.271 (3)	0.453 (3)	0.049*
C1	0.5306 (5)	0.4140 (3)	0.3481 (3)	0.0380 (6)
C2	0.6351 (5)	0.4545 (3)	0.2256 (3)	0.0426 (7)
C3	0.5019 (7)	0.5837 (3)	0.1357 (3)	0.0520 (8)
H3	0.5711	0.6130	0.0536	0.062*
C4	0.2697 (7)	0.6709 (3)	0.1634 (3)	0.0539 (8)
C5	0.1706 (7)	0.6261 (3)	0.2857 (3)	0.0536 (8)
H5	0.0142	0.6822	0.3062	0.064*

C6	0.2985 (6)	0.5003 (3)	0.3774 (3)	0.0461 (7)
H6	0.2300	0.4724	0.4597	0.055*
C7	0.5218 (5)	0.1865 (3)	0.5227 (3)	0.0449 (7)
C8	0.7104 (6)	0.0592 (4)	0.6200 (3)	0.0590 (9)
H8A	0.8681	0.0901	0.6462	0.071*
H8B	0.7927	-0.0072	0.5812	0.071*
C9	0.8830 (7)	0.3623 (4)	0.1907 (3)	0.0569 (8)
H9A	1.0565	0.3590	0.2325	0.085*
H9B	0.9069	0.4011	0.1006	0.085*
H9C	0.8435	0.2681	0.2168	0.085*
C10	0.1310 (10)	0.8109 (4)	0.0632 (4)	0.0815 (12)
H10A	0.2775	0.8560	0.0104	0.122*
H10B	0.0287	0.8712	0.1032	0.122*
H10C	-0.0013	0.7944	0.0121	0.122*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0551 (6)	0.1112 (9)	0.0893 (8)	-0.0082 (5)	0.0147 (5)	0.0236 (6)
O1	0.0134 (9)	0.0749 (15)	0.0926 (17)	-0.0115 (9)	-0.0051 (10)	-0.0006 (13)
N1	0.0138 (9)	0.0512 (13)	0.0519 (13)	-0.0051 (9)	-0.0010 (9)	-0.0132 (11)
C1	0.0211 (12)	0.0446 (15)	0.0476 (15)	-0.0062 (10)	-0.0031 (10)	-0.0166 (12)
C2	0.0263 (13)	0.0534 (17)	0.0504 (15)	-0.0104 (11)	0.0017 (11)	-0.0213 (13)
C3	0.0456 (17)	0.0573 (18)	0.0484 (16)	-0.0122 (14)	-0.0006 (13)	-0.0141 (14)
C4	0.0493 (18)	0.0474 (17)	0.0599 (18)	-0.0044 (13)	-0.0087 (14)	-0.0160 (14)
C5	0.0394 (16)	0.0548 (18)	0.0628 (19)	0.0047 (13)	-0.0037 (13)	-0.0242 (15)
C6	0.0278 (13)	0.0567 (17)	0.0503 (16)	-0.0021 (12)	0.0016 (11)	-0.0195 (13)
C7	0.0174 (12)	0.0522 (16)	0.0586 (17)	-0.0060 (11)	-0.0004 (11)	-0.0147 (13)
C8	0.0233 (13)	0.0593 (19)	0.073 (2)	-0.0076 (12)	-0.0009 (13)	-0.0021 (16)
C9	0.0369 (16)	0.072 (2)	0.0603 (18)	-0.0050 (14)	0.0090 (14)	-0.0270 (16)
C10	0.087 (3)	0.059 (2)	0.075 (2)	0.006 (2)	-0.009 (2)	-0.0087 (19)

*Geometric parameters (Å, °)*

C11—C8	1.728 (3)	C5—C6	1.371 (4)
O1—C7	1.223 (3)	C5—H5	0.9300
N1—C7	1.333 (4)	C6—H6	0.9300
N1—C1	1.425 (3)	C7—C8	1.516 (4)
N1—H1N	0.83 (4)	C8—H8A	0.9700
C1—C2	1.389 (4)	C8—H8B	0.9700
C1—C6	1.392 (4)	C9—H9A	0.9600
C2—C3	1.390 (4)	C9—H9B	0.9600
C2—C9	1.506 (4)	C9—H9C	0.9600
C3—C4	1.390 (5)	C10—H10A	0.9600
C3—H3	0.9300	C10—H10B	0.9600
C4—C5	1.378 (5)	C10—H10C	0.9600
C4—C10	1.511 (5)		

C7—N1—C1	124.3 (2)	O1—C7—N1	123.9 (3)
C7—N1—H1N	119 (2)	O1—C7—C8	121.4 (3)
C1—N1—H1N	117 (2)	N1—C7—C8	114.6 (2)
C2—C1—C6	120.4 (3)	C7—C8—C11	112.3 (2)
C2—C1—N1	120.0 (2)	C7—C8—H8A	109.1
C6—C1—N1	119.6 (2)	C11—C8—H8A	109.1
C1—C2—C3	117.6 (3)	C7—C8—H8B	109.1
C1—C2—C9	121.6 (3)	C11—C8—H8B	109.1
C3—C2—C9	120.9 (3)	H8A—C8—H8B	107.9
C4—C3—C2	122.8 (3)	C2—C9—H9A	109.5
C4—C3—H3	118.6	C2—C9—H9B	109.5
C2—C3—H3	118.6	H9A—C9—H9B	109.5
C5—C4—C3	117.8 (3)	C2—C9—H9C	109.5
C5—C4—C10	120.9 (3)	H9A—C9—H9C	109.5
C3—C4—C10	121.2 (3)	H9B—C9—H9C	109.5
C6—C5—C4	121.2 (3)	C4—C10—H10A	109.5
C6—C5—H5	119.4	C4—C10—H10B	109.5
C4—C5—H5	119.4	H10A—C10—H10B	109.5
C5—C6—C1	120.3 (3)	C4—C10—H10C	109.5
C5—C6—H6	119.9	H10A—C10—H10C	109.5
C1—C6—H6	119.9	H10B—C10—H10C	109.5
C7—N1—C1—C2	-130.4 (3)	C3—C4—C5—C6	0.7 (5)
C7—N1—C1—C6	50.8 (4)	C10—C4—C5—C6	-179.0 (3)
C6—C1—C2—C3	0.7 (4)	C4—C5—C6—C1	-0.8 (5)
N1—C1—C2—C3	-178.1 (2)	C2—C1—C6—C5	0.1 (4)
C6—C1—C2—C9	-179.1 (3)	N1—C1—C6—C5	178.9 (3)
N1—C1—C2—C9	2.1 (4)	C1—N1—C7—O1	2.5 (5)
C1—C2—C3—C4	-0.9 (4)	C1—N1—C7—C8	-178.9 (3)
C9—C2—C3—C4	178.9 (3)	O1—C7—C8—C11	-25.2 (4)
C2—C3—C4—C5	0.2 (5)	N1—C7—C8—C11	156.2 (3)
C2—C3—C4—C10	179.9 (3)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N $\cdots$ O1 <sup>i</sup>	0.83 (4)	2.04 (4)	2.853 (3)	165 (3)

Symmetry code: (i)  $x+1, y, z$ .