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# 2-Chloro-*N*-(4-methylphenyl)acetamide

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**Key indicators**

Single-crystal X-ray study
*T* = 299 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.097
*wR* factor = 0.288
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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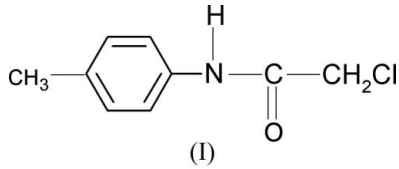
The structure of the title compound, $C_9H_{10}ClNO$, is closely related to those of 2-chloro-*N*-(4-nitrophenyl)acetamide and other related amides. The molecules are linked into zigzag chains through N—H···O hydrogen bonding.

## Comment

In the present work, the structure of 2-chloro-*N*-(4-methylphenyl)acetamide (4MP2CA), (I), has been determined as part of a study of the effect of substituents on the structures of *N*-aromatic amides (Gowda *et al.*, 2000, 2006, 2007*a*,*b*; Gowda, Kozisek *et al.*, 2007; Gowda, Paulus *et al.*, 2007).




(I)

The structure of 4MP2CA (Fig. 1) is closely related to those of 2-chloro-*N*-(4-nitrophenyl)acetamide (4NP2CA) (Gowda *et al.*, 2007*b*) and other related amides (Gowda *et al.*, 2000, 2007*a*). Although the two amides 4MP2CA and 4NP2CA are 4-substituted phenyl 2-chloroacetamides with electron-donating and withdrawing groups, respectively, there are no significant changes in the bond parameters of the amide group. The two compounds differ only slightly in the average C—C ring distances and the $C_{ring}$—N bond lengths [4MP2CA 1.418 (5) and 4NP2CA 1.401 (3) Å] (Gowda *et al.*, 2007*b*). In 4MP2CA, the molecules are linked into zigzag chains (Fig. 2) through N—H···O hydrogen bonds (Table 1).

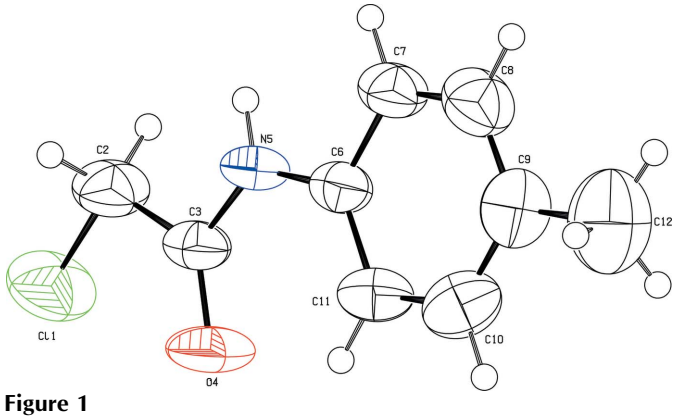



**Figure 1**
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radius.

## Experimental

The title compound was prepared according to the literature method of Gowda *et al.* (2003). The purity of the compound was checked by determining its melting point (429 K). It was characterized by recording its IR and NMR spectra (Gowda *et al.*, 2003). Single crystals were obtained by slow evaporation of an ethanol solution and used for X-ray diffraction studies at room temperature.

*Crystal data*

$C_9H_{10}ClNO$
$M_r$ = 183.63
Orthorhombic, *Pbca*
$a$ = 10.585 (2) Å
$b$ = 9.262 (4) Å
$c$ = 18.848 (9) Å
$V$ = 1847.8 (12) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 3.26 mm$^{-1}$
$T$ = 299 (2) K
0.75 × 0.18 × 0.18 mm

*Data collection*

Nonius CAD-4 diffractometer
Absorption correction: none
2368 measured reflections
1641 independent reflections
1171 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.188
3 standard reflections
frequency: 120 min
intensity decay: 5.2%

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.097
$wR(F^2)$ = 0.288
$S$ = 1.08
1641 reflections
114 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5*N*···O4$^{i}$ | 0.857 (10) | 2.014 (15) | 2.845 (4) | 163 (4) |

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

C-bound H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (aromatic), 0.96 (methyl) or 0.97 Å ($CH_2$) and with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C). The H atom attached to nitrogen was freely refined.

Data collection: *CAD-4 EXPRESS* (Nonius, 1996); cell refinement: *CAD-4 EXPRESS*; 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) and *ORTEP-3* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

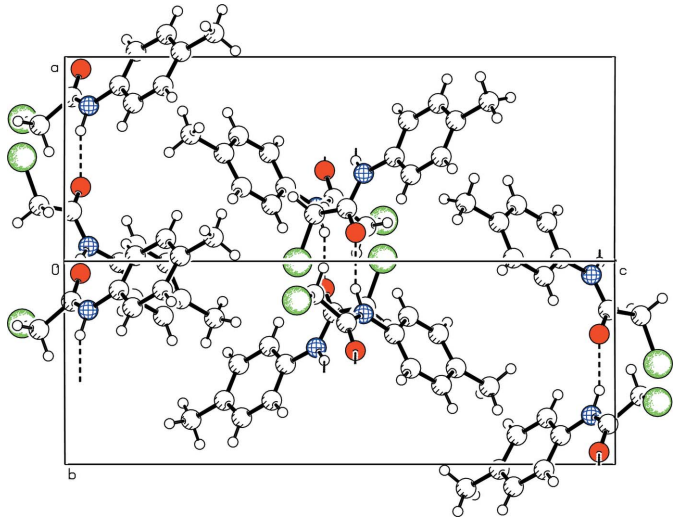



**Figure 2**
Packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

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