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2-Chloro-*N*-(4-nitrophenyl)acetamide

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In the crystal structure of the title compound, $C_8H_7ClN_2O_3$, the molecules are linked into chains by N—H···O hydrogen bonds.

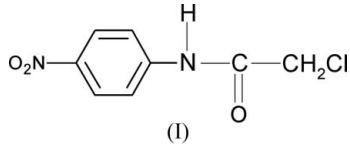
Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.101
Data-to-parameter ratio = 10.8

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

Comment

As part of a study on the systematization of the crystal structures of acetanilides (Gowda *et al.*, 2006; Gowda, Kozisek *et al.*, 2007; Gowda, Foro & Fuess, 2007), the structure of 2-chloro-*N*-(4-nitrophenyl)acetamide (4NP2CA), (I), has been determined to explore the effects of polar substituent groups on the structure of *N*-aromatic amides. In 4NP2CA, the amide H atom is involved in intermolecular hydrogen bonding with the O atom (Table 1).



(I)

Experimental

The title compound, (I), was prepared according to a literature method (Gowda & Weiss, 1994). The purity of the compound was checked by determining its melting point. It was characteried by recording its IR and NQR spectra (Gowda & Weiss, 1994). Single crystals of the title compound were obtained from an ethanol solution.

Crystal data

$C_8H_7ClN_2O_3$
M_r = 214.61
Orthorhombic, *Pbca*
a = 9.460 (1) Å
b = 20.194 (3) Å
c = 9.496 (1) Å
V = 1814.1 (4) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 3.63 mm^{-1}
T = 299 (2) K
0.33 × 0.30 × 0.05 mm

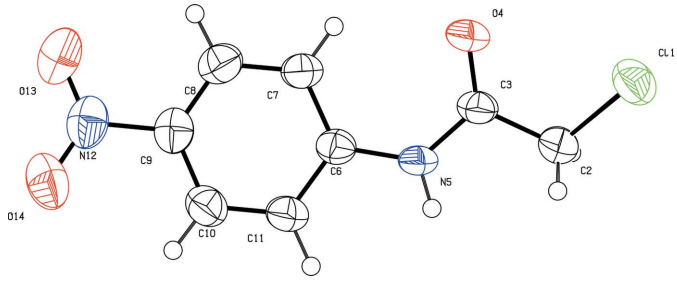


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.353, T_{max} = 0.834
5404 measured reflections
1610 independent reflections
1294 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
3 standard reflections
frequency: 120 min
intensity decay: 3.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.04
1610 reflections
149 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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}	0.845 (10)	2.040 (12)	2.840 (2)	158 (2)

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

H atoms bonded to C were positioned geometrically and treated as riding, with C—H = 0.93 (aromatic) or 0.97 Å (CH_2), and with U_{iso}(H) = 1.2U_{eq}(C). The coordinates of the H atom bonded to nitrogen were refined with U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *CAD-4-PC* (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*.

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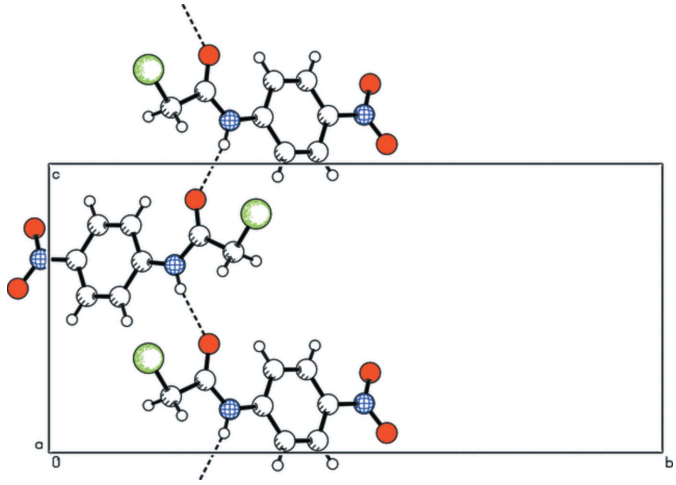

Figure 2
Partial packing diagram of the title compound, viewed in the *bc* plane. Hydrogen bonds are shown as dashed lines.

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