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3-Chloropropionamide

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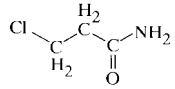
The crystal structure of 3-chloropropionamide, C_3H_6ClNO, (I), was determined in order to obtain coordinates for molecular-orbital calculations. Intermolecular N—H···O and C—H···O hydrogen bonds link the molecules into continuous two-dimensional sheets parallel to the (100) plane. The bond distances are C—Cl 1.793 (3), C═O 1.233 (3) and C—N 1.320 (3) Å.



(I)

Experimental

Crystals of the title compound were grown from an aqueous solution.

Crystal data

C_3H_6ClNO
M_r = 107.54
Monoclinic, $P2_1/c$
a = 6.880 (2) Å
b = 8.201 (3) Å
c = 9.298 (2) Å
β = 105.59 (1)°
V = 505.3 (2) Å^3
Z = 4
D_x = 1.414 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.2–15.0°
μ = 0.609 mm^{-1}
T = 296.2 K
Prismatic, colourless
0.20 × 0.15 × 0.15 mm

Data collection

Rigaku AFC-5R diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.882, T_{max} = 0.913
1306 measured reflections
1153 independent reflections
757 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.007
θ_{max} = 27.51°
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 10$
$l = -12 \rightarrow 0$
3 standard reflections
every 150 reflections
intensity decay: 3.9%

Refinement

Refinement on F^2
$R(F)$ = 0.0354
$wR(F^2)$ = 0.1085
S = 0.960
849 reflections
80 parameters
All H-atom parameters refined
$w = 1/\{\sigma^2(F_o^2) + [0.08600(\mathrm{Max}(F_o^2,0) + 2F_c^2)/3]^2\}$
$(\Delta/\sigma)_{max}$ = 0.0065
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: Zachariasen (1967), type 2, Gaussian isotropic
Extinction coefficient: 0.01 (1)

The H atoms were located from difference maps and were refined with isotropic displacement parameters.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1990); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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