

M. Khawar Rauf,^{a*} Amin Badshah,^a Michael Bolte^b and Aamer Saeed^a

^aDepartment of Chemistry, Quaid-I-Azam University, Islamabad, Pakistan, and ^bInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Strasse 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail: aminbadshah@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.030
 wR factor = 0.078
Data-to-parameter ratio = 14.3

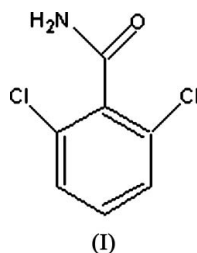
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

2,6-Dichlorobenzamide

The amide group of the title compound, $\text{C}_7\text{H}_5\text{Cl}_2\text{NO}$, forms a dihedral angle of $76.64(5)^\circ$ with the plane of the benzene ring. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link molecules, forming one-dimensional chains in the c -axis direction.

Comment

Benzamide and its derivatives have attracted the attention of researchers in a number of fields over the last two decades; *e.g.* α,β -unsaturated ketobenzamides are used as the inhibitors of human rhinovirus 3C protease (Reich *et al.*, 2000) and orally active benzamides are used as antipsychotic agents with affinity for dopamine D2 serotonin 5-HT1A and adrenergic receptors (Reitz *et al.*, 1998). In addition, a series of substituted {4-[4-(1,2-benzisothiazol-3-yl)piperazin-1-yl]butyl}benzamide derivatives have been prepared and evaluated as potential atypical antipsychotic agents (Norman *et al.*, 1996).



The title compound, (I) (Fig. 1), is a chemical precursor in the manufacture of compounds such as insecticides, pesticides, phenobarbital, antipsychotic agents and various dyes. It is also an important metabolite of chlobenil (2,6-dichlorobenzonitrile), which is used as a herbicide (Cox, 1997). The bond lengths and angles in (I) are as expected (Table 1); for example, the $\text{C7}-\text{O1}$ bond shows the expected double-bond character and the shorter than normal $\text{C7}-\text{N}$ bond also indicates some double-bond character, as in the structure of benzamide (Blake & Small, 1972; Gao *et al.*, 1991); the Cl substituents at C2 and C6 have no significant effect on these bond lengths. The amide group forms a dihedral angle of $76.64(5)^\circ$ with the plane of the aromatic ring. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link molecules, forming one-dimensional chains in the c -axis direction (Table 2 and Fig. 2).

Experimental

The title compound was prepared according to a standard method given in the literature (Finan & Fothergill, 1962). A mixture of 2,6-

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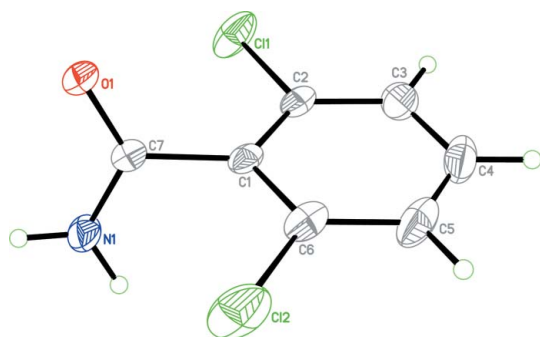


Figure 1

A perspective view of the title compound, showing displacement ellipsoids at the 50% probability level.

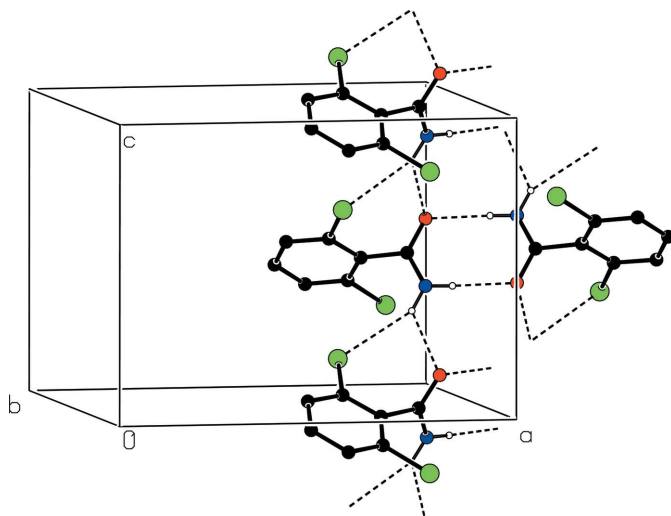


Figure 2

Partial packing plot (Spek, 2003), showing hydrogen bonds as dashed lines. Color codes: green Cl, red O and blue N.

dichlorobenzoyl chloride (2.1 g, 10 mmol) and ammonium acetate (0.8 g, 10 mmol) in acetone (20 ml) was stirred vigorously for 1–2 h. The reaction mixture was filtered and the filtrate was evaporated to dryness under vacuum on a rotary evaporator. The solid residue was crystallized from hot toluene to give colorless needles of the title compound, with an overall yield of 85%.

Crystal data

$C_7H_5Cl_2NO$
 $M_r = 190.02$
 Orthorhombic, *Pbcn*
 $a = 12.7941$ (9) Å
 $b = 13.5868$ (8) Å
 $c = 9.5283$ (6) Å
 $V = 1656.31$ (18) Å³
 $Z = 8$
 $D_x = 1.524$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 17745 reflections
 $\theta = 3.5$ – 25.8°
 $\mu = 0.72$ mm⁻¹
 $T = 173$ (2) K
 Needle, colorless
 $0.42 \times 0.20 \times 0.20$ mm

Data collection

Stoe IPDS-II two-circle diffractometer
 ω scans
 Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)
 $T_{min} = 0.752$, $T_{max} = 0.869$
 16372 measured reflections

1556 independent reflections
 1486 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.056$
 $\theta_{max} = 25.6^\circ$
 $h = -15 \rightarrow 15$
 $k = -16 \rightarrow 13$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.078$
 $S = 1.11$
 1556 reflections
 109 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 0.9959P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.30$ e Å⁻³
 $\Delta\rho_{min} = -0.38$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0098 (13)

Table 1

Selected geometric parameters (Å, °).

Cl1—C2	1.7463 (16)	N1—C7	1.327 (2)
Cl2—C6	1.7444 (18)	O1—C7	1.2444 (18)
O1—C7—N1	123.92 (14)	N1—C7—C1	116.44 (13)
O1—C7—C1	119.64 (13)		

Table 2

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>
N1—H1A···Cl1 ⁱ	0.91 (2)	2.78 (2)	3.5936 (15)	150.4 (18)
N1—H1A···O1 ⁱ	0.91 (2)	2.32 (2)	2.9728 (18)	128.5 (18)
N1—H1B···O1 ⁱⁱ	0.87 (2)	2.08 (2)	2.9491 (18)	178 (2)

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

H atoms were located in a difference map. Those bonded to C atoms were refined with fixed individual displacement parameters [$U_{iso}(H) = 1.2U_{eq}(C)$] using a riding model, with C—H = 0.95 Å. The H atoms bonded to N1 were refined isotropically.

Data collection: X-AREA (Stoe & Cie, 2001); cell refinement: X-AREA; data reduction: X-AREA; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Sheldrick, 1991) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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