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4-Chloro-2-nitroaniline

Yuan Yang,[a] Ulli Englert[b] and Qi Li[a]*

[a]College of Chemistry, Beijing Normal University, Xinjiekouwai Street 19, Beijing 100875, People's Republic of China, and [b]Institut für Anorganische Chemie, RWTH Aachen, Prof.-Pirlet-Strasse 1, 52074 Aachen, Germany

Correspondence e-mail: qili@bnu.edu.cn

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Key indicators

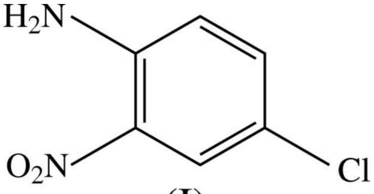
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.109
Data-to-parameter ratio = 11.6

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

The title molecule, $C_6H_5ClN_2O_2$, crystallizes with two molecules in the asymmetric unit. Both residues are planar with an intramolecular hydrogen bond between the amino and nitro groups. Two intermolecular hydrogen bonds connect the crystallographically independent molecules into a dimer. Dimers are linked by N—H···O hydrogen bonding into a one-dimensional ribbon.

Comment

4-Chloro-2-nitroaniline, (I), is well known as an intermediate in organic synthesis (Mosher *et al.*, 1947; Lebegue *et al.*, 2005). It has also received increasing attention due to its toxicity (Rolf *et al.*, 2005). Structural investigations on several chloronitroanilines, namely 2-chloro-4-nitroaniline (McPhail & Sim, 1965), 4,5-dichloro-2-nitroaniline (Doyle, 1999) and 5-chloro-2-nitroaniline (Ng, 2005) have been reported. Here we report the crystal structure of 4-chloro-2-nitroaniline; the structure of its cocrystal with $[Cd(phen)_3](BF_4)_2$ (phen is 1,10-phenanthroline) was reported previously (Chen *et al.*, 1998).



(I)

The asymmetric unit of (I) contains two independent molecules; in each molecule, an intramolecular hydrogen bond between an amino H atom and the nearest oxygen of the nitro group occurs. The independent molecules are joined into a dimer *via* two intermolecular hydrogen bonds in which the amino H acts as a double donor to the two O atoms of a nitro group (Fig. 1 and Table 1). Intermolecular N—H···O hydrogen bonding connects dimers in a head-to-tail fashion into infinite chains (Fig. 2) in the [110] and [$\bar{1}$10] directions (Fig. 3). The shortest interchain contacts of 3.129 (4) Å involve chlorine and nitro O atoms. This distance and the C—Cl···O angle of 161.7 (3)° compare well with values reported by Lommerse *et al.* (1996).

Experimental

The commercially available title compound was recrystallized from dichloromethane. After two days, yellow needle-shaped crystals appeared.

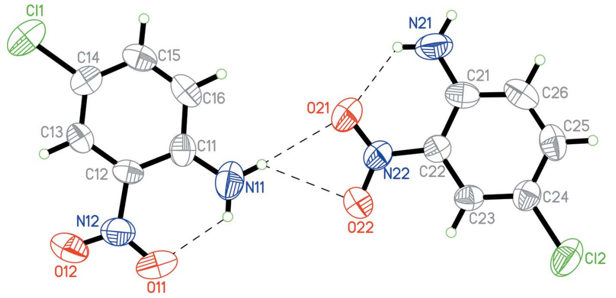


Figure 1
The structure of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate hydrogen bonds.

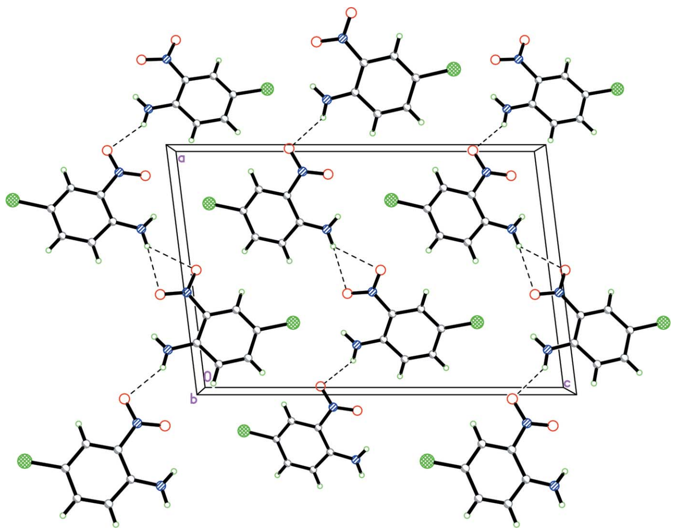


Figure 2
View of the packing along the *b* axis. Dashed lines indicate intermolecular hydrogen bonds.

Crystal data

$C_6H_5ClN_2O_2$
$M_r = 172.57$
Monoclinic, *Pc*
$a = 11.272$ (3) Å
$b = 3.8023$ (11) Å
$c = 17.016$ (5) Å
$\beta = 97.051$ (8)°
$V = 723.8$ (4) Å^3
$Z = 4$
$D_x = 1.584$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.47$ mm^{-1}
$T = 293$ (2) K
Needle, yellow
0.31 × 0.14 × 0.08 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.867$, $T_{\max} = 0.963$
4637 measured reflections
2318 independent reflections
1544 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 28.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.109$
$S = 1.00$
2318 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Absolute structure: Flack (1983), with 517 Friedel pairs
Flack parameter: 0.03 (8)

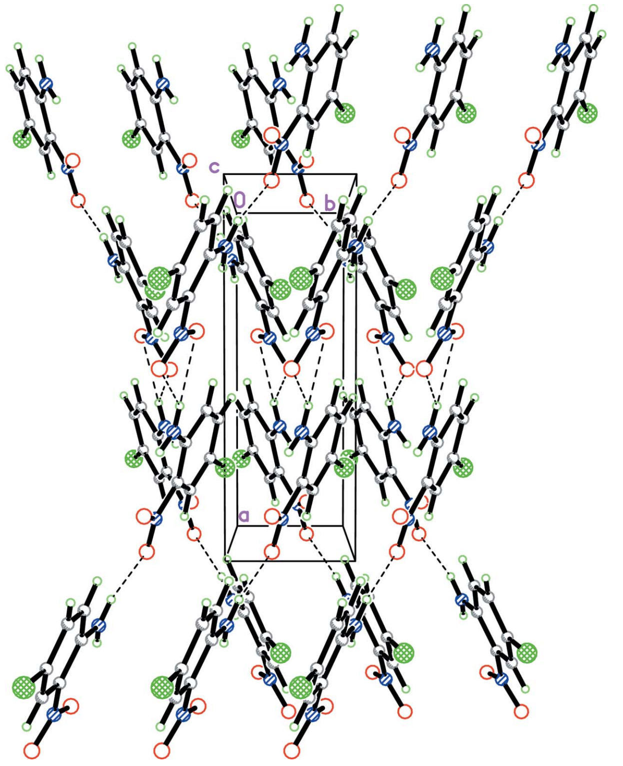


Figure 3
View of the packing along the *c* axis. Dashed lines indicate intermolecular hydrogen bonds.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*A*···O11	0.86	2.04	2.645 (4)	127
N21—H21*B*···O21	0.86	2.03	2.642 (3)	127
N11—H11*B*···O21	0.86	2.36	3.218 (4)	176
N11—H11*B*···O22	0.86	2.50	3.138 (4)	131
N21—H21*A*···O12$^{\rm i}$	0.86	2.26	3.017 (3)	146

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

All H atoms were positioned geometrically, with C—H = 0.93 Å and N—H = 0.86 Å, and refined as rifding with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS* in *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXL* in *SHELXTL*; molecular graphics: SHELXP in *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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