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1-Chloromethyl-4-nitrobenzene

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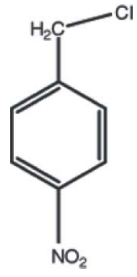
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.103; data-to-parameter ratio = 18.2.

In the title compound, $C_7H_6ClNO_2$, the nitro group is almost coplanar with the aromatic ring [dihedral angle = 2.9 (2)°], but the Cl atom deviates from the ring plane by 1.129 (1) Å. In the crystal, molecules are linked by weak C—H···O interactions to generate chains.

Related literature

For background on the toxicity of nitro-aromatic compounds, see: Moreno *et al.* (1986). For the synthesis of the title compound, see: Livermore & Sealock (1947). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_7H_6ClNO_2$
M_r = 171.58
Orthorhombic, $P2_12_12_1$
a = 4.7434 (1) Å
b = 6.4189 (2) Å
c = 24.9413 (11) Å
V = 759.40 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 296 K
0.35 × 0.11 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
4389 measured reflections
1816 independent reflections
1586 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.04
1816 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 662 Freidel pairs
Flack parameter: 0.02 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7B···O1^{i}	0.97	2.48	3.396 (3)	158

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PARST* (Nardelli, 1983) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5491).

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supplementary materials

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1-Chloromethyl-4-nitrobenzene

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Comment

The irreversible binding of the reductive intermediates of nitroaromatic compounds to protein and DNA is thought to be responsible for the carcinogenicity and mutagenicity of this class of compounds. Several studies revealed that some nitro radical metabolites with special features are expected to decompose to form neutral carbon-centered free radicals with not net reduction of the nitro group occurring. The radicals anions of *p*-and *o*-nitrobenzyl chloride are known to expel chloride to form the corresponding carbon-centered nitrobenzyl radicals with rate constants of 1 × 104 and 4 × 103 s^{-1}. Such species are highly reactive and could account for the unusual cytotoxicity of these nitrocompounds (Moreno *et al.*, 1986). This structural report on 1-(chloromethyl)-4-nitrobenzene (*p*-nitrobenzyl chloride) might be helpful to carry out such studies on these nitroaromatic compounds in future.

The title molecule (I), (Fig. 1), is non-planar and the dihedral angle between the plane of the NO_2 group and benzene (C1–C6) ring is 2.9 (2)°, while the C5—C4—C7—Cl1 torsion angle is 83.8 (2)°. In (I), the bond lengths (Allen *et al.*, 1987) and angles have values within the normal ranges.

In the crystal structure, there is no classic hydrogen bonds. A weak intermolecular C—H···O interaction contrubutes to the stability of the structure (Table 1, Fig. 2).

Experimental

The title *p*-nitrobenzyl chloride was prepared by adding 5.3 ml of benzyl chloride slowly and with stirring to 27.5 ml of a mixture of equal parts of concentrated nitric and sulfuric acids cooled to 283 K. The temperature rose to 303 K during the 10 min required for the addition. The mixture was stirred for 30 min and then poured into 50 g of crushed ice. The crude material was recrystallized from ethanol. Product obtained was dissolved in ethanol and crystallized by slow evaporation of the solvent to yield colourless needles of (I) in an over-all yield of 46% (Livermore & Sealock, 1947).

Refinement

H atoms were positioned geometrically (C—H = 0.93 and 0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

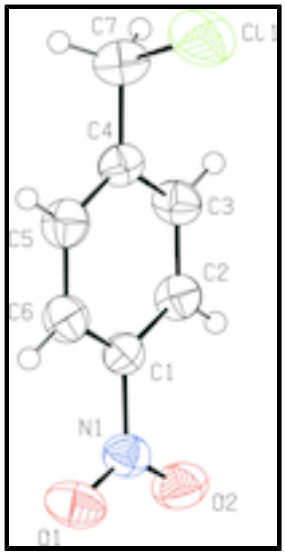

Fig. 1. View of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

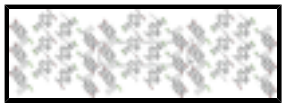

Fig. 2. The crystal packing and the hydrogen bonding of (I) viewed down the *a*-axis. H-atoms not involved in hydrogen bonds have been omitted for clarity.

1-Chloromethyl-4-nitrobenzene

Crystal data

$C_7H_6ClNO_2$	$F(000) = 352$
$M_r = 171.58$	$D_x = 1.501$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 1957 reflections
$a = 4.7434$ (1) Å	$\theta = 3.3$–$26.7°$
$b = 6.4189$ (2) Å	$\mu = 0.45$ mm^{-1}
$c = 24.9413$ (11) Å	$T = 296$ K
$V = 759.40$ (4) Å^3	Needle, colourless
$Z = 4$	0.35 × 0.11 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer	1586 reflections with $I > 2\sigma(I)$
Radiation source: sealed tube	$R_{int} = 0.018$
graphite	$\theta_{max} = 28.3°$, $\theta_{min} = 3.3°$
φ and ω scans	$h = -5 \rightarrow 6$
4389 measured reflections	$k = -8 \rightarrow 5$
1816 independent reflections	$l = -33 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.1709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
1816 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
100 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 662 Freidel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (11)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.75015 (18)	0.45250 (12)	0.22343 (3)	0.0812 (3)
O1	1.4188 (4)	−0.3381 (3)	0.07002 (7)	0.0621 (6)
O2	1.4761 (4)	−0.0854 (3)	0.01453 (7)	0.0601 (6)
N1	1.3647 (3)	−0.1634 (3)	0.05351 (7)	0.0434 (5)
C1	1.1532 (4)	−0.0398 (3)	0.08269 (7)	0.0364 (5)
C2	1.0829 (4)	0.1540 (3)	0.06377 (7)	0.0421 (6)
C3	0.8901 (4)	0.2704 (3)	0.09215 (8)	0.0437 (6)
C4	0.7690 (4)	0.1928 (3)	0.13883 (7)	0.0393 (5)
C5	0.8402 (5)	−0.0046 (3)	0.15629 (8)	0.0472 (6)
C6	1.0341 (5)	−0.1235 (3)	0.12836 (8)	0.0459 (6)
C7	0.5663 (5)	0.3213 (4)	0.17034 (8)	0.0533 (7)
H2	1.16370	0.20560	0.03250	0.0510*
H3	0.84040	0.40230	0.08000	0.0520*
H5	0.75690	−0.05800	0.18710	0.0570*
H6	1.08280	−0.25630	0.14000	0.0550*
H7A	0.42040	0.23280	0.18530	0.0640*
H7B	0.47710	0.42290	0.14710	0.0640*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0957 (5)	0.0831 (5)	0.0647 (4)	0.0041 (4)	0.0047 (4)	−0.0299 (3)
O1	0.0677 (11)	0.0514 (9)	0.0671 (10)	0.0222 (8)	−0.0024 (8)	0.0041 (8)
O2	0.0584 (10)	0.0629 (11)	0.0591 (9)	0.0072 (8)	0.0175 (8)	0.0010 (8)
N1	0.0412 (8)	0.0450 (9)	0.0440 (8)	0.0046 (8)	−0.0047 (7)	−0.0051 (7)
C1	0.0336 (8)	0.0382 (9)	0.0374 (8)	0.0008 (7)	−0.0048 (7)	−0.0001 (7)
C2	0.0446 (10)	0.0451 (11)	0.0366 (9)	0.0024 (9)	0.0012 (7)	0.0076 (8)
C3	0.0496 (11)	0.0409 (10)	0.0406 (9)	0.0079 (9)	−0.0016 (8)	0.0079 (8)
C4	0.0362 (9)	0.0460 (10)	0.0357 (8)	0.0024 (9)	−0.0033 (7)	−0.0008 (7)
C5	0.0526 (11)	0.0495 (12)	0.0394 (9)	−0.0012 (9)	0.0046 (8)	0.0080 (8)
C6	0.0500 (11)	0.0405 (10)	0.0471 (10)	0.0015 (9)	0.0001 (9)	0.0084 (8)
C7	0.0510 (12)	0.0613 (13)	0.0475 (11)	0.0111 (12)	0.0033 (9)	−0.0004 (10)

Geometric parameters (Å, °)

Cl1—C7	1.795 (2)	C4—C7	1.491 (3)
O1—N1	1.222 (3)	C5—C6	1.383 (3)
O2—N1	1.215 (2)	C2—H2	0.9300
N1—C1	1.472 (3)	C3—H3	0.9300
C1—C2	1.372 (3)	C5—H5	0.9300
C1—C6	1.380 (3)	C6—H6	0.9300
C2—C3	1.377 (3)	C7—H7A	0.9700
C3—C4	1.391 (3)	C7—H7B	0.9700
C4—C5	1.382 (3)		
O1—N1—O2	123.83 (19)	C1—C2—H2	121.00
O1—N1—C1	118.12 (17)	C3—C2—H2	121.00
O2—N1—C1	118.05 (18)	C2—C3—H3	120.00
N1—C1—C2	118.98 (16)	C4—C3—H3	120.00
N1—C1—C6	118.51 (17)	C4—C5—H5	120.00
C2—C1—C6	122.51 (18)	C6—C5—H5	120.00
C1—C2—C3	118.48 (17)	C1—C6—H6	121.00
C2—C3—C4	120.69 (18)	C5—C6—H6	121.00
C3—C4—C5	119.43 (18)	Cl1—C7—H7A	110.00
C3—C4—C7	120.64 (18)	Cl1—C7—H7B	110.00
C5—C4—C7	119.93 (18)	C4—C7—H7A	110.00
C4—C5—C6	120.65 (18)	C4—C7—H7B	110.00
C1—C6—C5	118.22 (18)	H7A—C7—H7B	108.00
Cl1—C7—C4	109.58 (16)		
O1—N1—C1—C2	−177.90 (18)	C1—C2—C3—C4	−0.2 (3)
O1—N1—C1—C6	2.4 (3)	C2—C3—C4—C5	−1.0 (3)
O2—N1—C1—C2	2.4 (3)	C2—C3—C4—C7	178.30 (19)
O2—N1—C1—C6	−177.28 (19)	C3—C4—C5—C6	1.2 (3)
N1—C1—C2—C3	−178.37 (17)	C7—C4—C5—C6	−178.1 (2)
C6—C1—C2—C3	1.3 (3)	C3—C4—C7—Cl1	−95.5 (2)
N1—C1—C6—C5	178.55 (18)	C5—C4—C7—Cl1	83.8 (2)

C2—C1—C6—C5	−1.1 (3)	C4—C5—C6—C1	−0.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7B···O1^{i}	0.97	2.48	3.396 (3)	158

Symmetry codes: (i) *x*−1, *y*+1, *z*.

Fig. 1

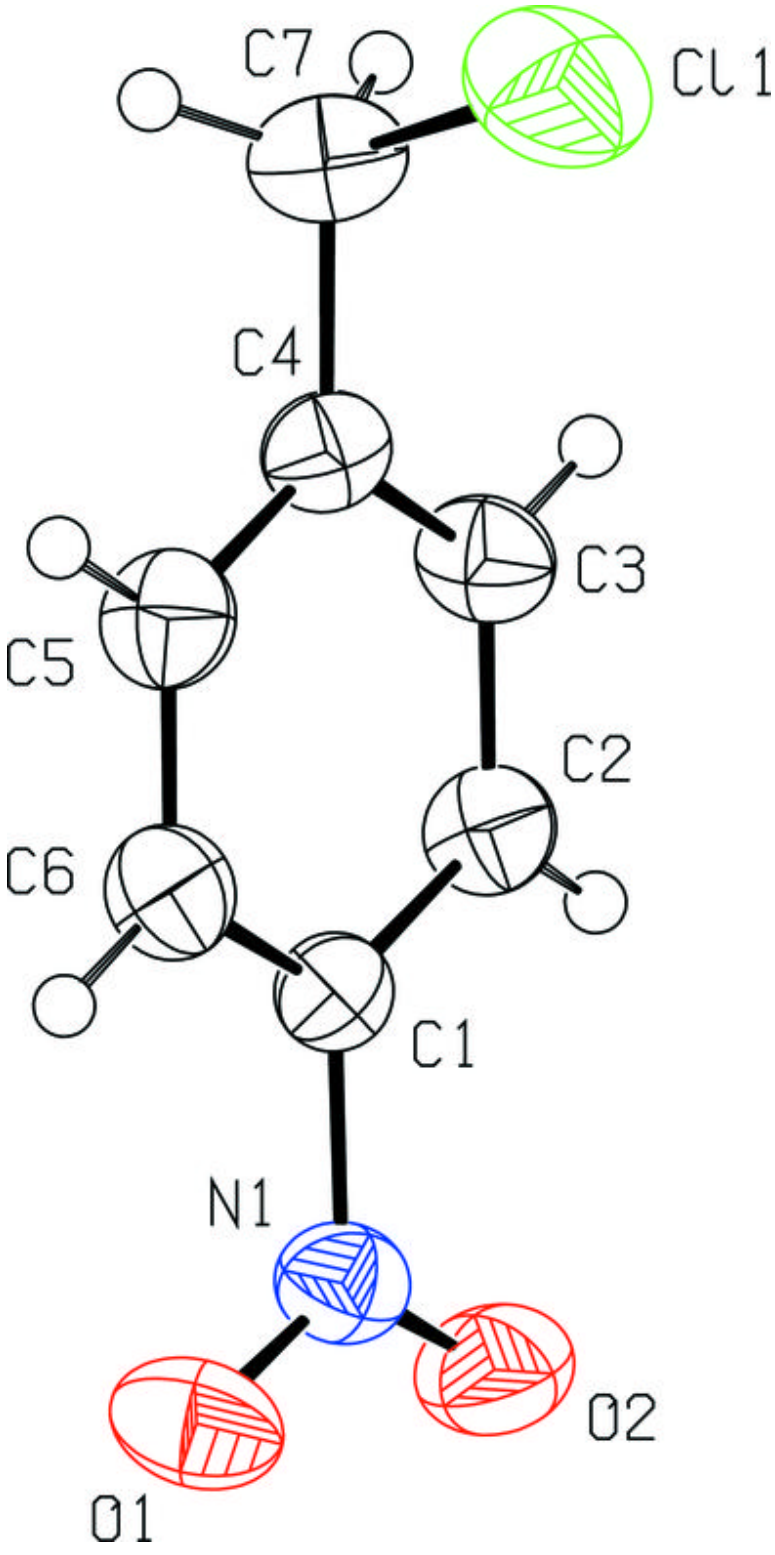

Fig. 2