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4-Chloro-2-nitro-1-(2-phenylethyl)benzene

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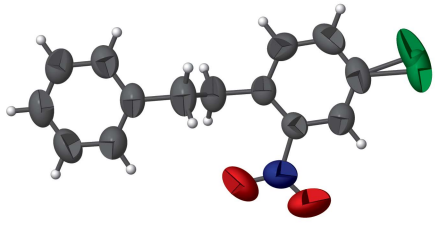
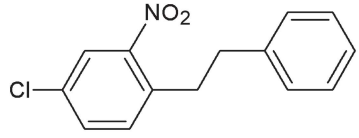
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{12}ClNO_2$, the dihedral angle between the aromatic rings is 6.09 (17)° and the $C_{ar}—C—C—C_{ar}$ torsion angle is −179.4 (3)°. The nitro group is close to coplanar with its attached ring [dihedral angle = 7.9 (2)°] and the Cl atom is disordered over two adjacent sites in a 0.54 (4):0.46 (4) ratio. In the crystal, C—H···O hydrogen bonds link the molecules into *C*(6) [001] chains.

3D view



Chemical scheme



Structure description

As part of out interest in the synthesis and crystal structures of 4-chloronitrobenzene derivatives, the title compound (Fig. 1) is reported here.

The dihedral angle between the aromatic rings is 6.09 (17)° and the C6—C7—C8—C9 torsion angle is −179.4 (3)°. The nitro group is close to being coplanar with its attached ring [dihedral angle = 7.9 (2)°]. In the crystal, C—H···O hydrogen bonds (Table 1) link the molecules into *C*(6) [001] chains (Fig. 2).

Synthesis and crystallization

4-Chloronitrobenzene (1.57 g, 0.01 mol) was dissolved in 25 ml of ethanol and styrene (1.04 g, 0.01 mol) was dissolved in 25 ml of ethanol. The solutions were mixed and stirred in a beaker at 30° C for 1 h. The mixture was kept aside for two days at room temperature. The formed product was filtered and dried in a vacuum desiccator over phosphorous pentoxide. The product was recrystallized from toluene solution by slow evaporation (m.p. 399–401 K) in the form of colourless blocks.

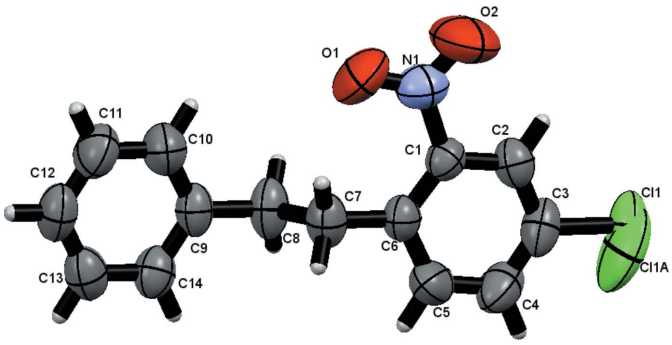


Figure 1
A view of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

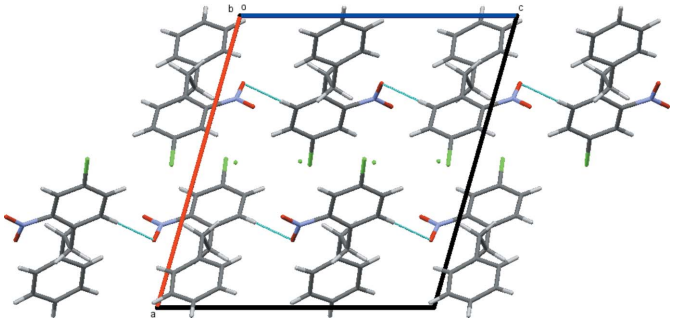


Figure 2
A view along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are drawn as dashed lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The Cl atom is disordered over two adjacent sites in a 0.54 (4):0.46 (4) ratio.

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.54	3.462 (5)	175

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}ClNO_2$
M_r	261.70
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	14.201 (3), 7.3285 (12), 12.974 (4)
β (°)	105.89 (2)
V (Å^3)	1298.6 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.19 × 0.18 × 0.15
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.947, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13474, 2554, 1389
R_{int}	0.095
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.220, 1.04
No. of reflections	2554
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.18

Computer programs: *CrystalClear SM Expert* (Rigaku, 2011), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2017). **2**, x170547 [https://doi.org/10.1107/S2414314617005478]

4-Chloro-2-nitro-1-(2-phenylethyl)benzene

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4-Chloro-2-nitro-1-(2-phenylethyl)benzene

Crystal data

$C_{14}H_{12}ClNO_2$
M_r = 261.70
Monoclinic, $P2_1/c$
a = 14.201 (3) Å
b = 7.3285 (12) Å
c = 12.974 (4) Å
β = 105.89 (2)°
V = 1298.6 (5) Å^3
Z = 4
$F(000)$ = 544
D_x = 1.338 Mg m^{-3}
Melting point: 399 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2554 reflections
θ = 3–52°
μ = 0.29 mm^{-1}
T = 293 K
Block, colourless
0.19 × 0.18 × 0.15 mm

Data collection

Rigaku Saturn724+ diffractometer
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.947, T_{max} = 0.960
13474 measured reflections
2554 independent reflections
1389 reflections with $I > 2\sigma(I)$
R_{int} = 0.095
θ_{max} = 26.0°, θ_{min} = 3.0°
h = −17→17
k = −9→9
l = −16→15
2554 standard reflections

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.220
S = 1.04
2554 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 0.1859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.4908 (4)	−0.3295 (6)	0.5958 (8)	0.101 (2)	0.54 (4)
O1	0.7685 (3)	0.1384 (5)	0.4195 (2)	0.1401 (13)	
O2	0.6890 (3)	−0.0951 (6)	0.3611 (3)	0.1827 (18)	
N1	0.7168 (2)	0.0150 (5)	0.4293 (2)	0.0921 (9)	
C1	0.6844 (2)	−0.0018 (4)	0.5279 (2)	0.0626 (8)	
C2	0.6156 (2)	−0.1349 (4)	0.5248 (3)	0.0736 (9)	
H2	0.5927	−0.2064	0.4639	0.088*	
C3	0.5815 (2)	−0.1608 (4)	0.6111 (3)	0.0827 (10)	
C4	0.6153 (3)	−0.0577 (5)	0.6996 (3)	0.1003 (12)	
H4	0.5917	−0.0757	0.7590	0.120*	
C5	0.6847 (3)	0.0743 (5)	0.7018 (3)	0.0945 (11)	
H5	0.7069	0.1447	0.7633	0.113*	
C6	0.7228 (2)	0.1067 (4)	0.6156 (2)	0.0675 (8)	
C7	0.7986 (2)	0.2541 (4)	0.6279 (3)	0.0842 (10)	
H7A	0.8439	0.2210	0.5871	0.101*	
H7B	0.8354	0.2624	0.7027	0.101*	
C8	0.7545 (2)	0.4399 (4)	0.5905 (3)	0.0904 (11)	
H8A	0.7173	0.4317	0.5158	0.108*	
H8B	0.7098	0.4740	0.6318	0.108*	
C9	0.8315 (2)	0.5853 (4)	0.6023 (3)	0.0736 (9)	
C10	0.8801 (3)	0.6110 (5)	0.5244 (3)	0.0948 (11)	
H10	0.8641	0.5391	0.4630	0.114*	
C11	0.9520 (3)	0.7420 (6)	0.5368 (3)	0.1023 (12)	
H11	0.9830	0.7582	0.4829	0.123*	
C12	0.9783 (3)	0.8470 (5)	0.6250 (3)	0.0918 (11)	
H12	1.0273	0.9342	0.6325	0.110*	
C13	0.9318 (3)	0.8232 (4)	0.7035 (3)	0.0874 (11)	
H13	0.9491	0.8954	0.7647	0.105*	
C14	0.8591 (2)	0.6926 (4)	0.6925 (3)	0.0790 (9)	
H14	0.8286	0.6773	0.7468	0.095*	
Cl1A	0.5021 (10)	−0.3187 (16)	0.634 (3)	0.169 (4)	0.46 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0740 (19)	0.069 (3)	0.161 (4)	−0.0124 (12)	0.031 (2)	0.015 (3)
O1	0.171 (3)	0.143 (3)	0.132 (2)	−0.030 (2)	0.084 (2)	0.025 (2)
O2	0.236 (4)	0.223 (4)	0.114 (2)	−0.069 (4)	0.089 (3)	−0.069 (3)
N1	0.100 (2)	0.102 (2)	0.080 (2)	0.0064 (18)	0.0352 (17)	−0.0007 (18)
C1	0.0647 (18)	0.0570 (16)	0.0696 (18)	0.0061 (13)	0.0240 (14)	0.0066 (14)
C2	0.0651 (19)	0.0626 (18)	0.090 (2)	0.0003 (14)	0.0151 (17)	−0.0029 (16)
C3	0.069 (2)	0.0570 (19)	0.130 (3)	0.0019 (15)	0.041 (2)	0.0143 (19)
C4	0.133 (3)	0.076 (2)	0.118 (3)	0.008 (2)	0.077 (3)	0.013 (2)
C5	0.142 (3)	0.068 (2)	0.080 (2)	−0.004 (2)	0.040 (2)	−0.0088 (17)
C6	0.0700 (19)	0.0542 (17)	0.077 (2)	−0.0004 (14)	0.0180 (16)	0.0046 (15)

C7	0.074 (2)	0.065 (2)	0.106 (2)	−0.0045 (16)	0.0099 (18)	0.0105 (18)
C8	0.076 (2)	0.0575 (19)	0.134 (3)	−0.0004 (15)	0.022 (2)	0.0109 (19)
C9	0.0648 (19)	0.0514 (17)	0.101 (2)	0.0005 (14)	0.0160 (17)	0.0065 (17)
C10	0.105 (3)	0.080 (2)	0.100 (3)	−0.018 (2)	0.030 (2)	−0.0054 (19)
C11	0.102 (3)	0.096 (3)	0.118 (3)	−0.020 (2)	0.046 (2)	0.010 (3)
C12	0.078 (2)	0.073 (2)	0.116 (3)	−0.0160 (17)	0.014 (2)	0.016 (2)
C13	0.086 (3)	0.066 (2)	0.100 (3)	−0.0012 (17)	0.008 (2)	0.0001 (18)
C14	0.075 (2)	0.063 (2)	0.101 (2)	0.0045 (16)	0.0282 (18)	0.0085 (18)
Cl1A	0.103 (4)	0.162 (6)	0.252 (12)	−0.030 (3)	0.068 (5)	0.083 (5)

Geometric parameters (Å, º)

Cl1—C3	1.757 (6)	C7—H7B	0.9700
O1—N1	1.193 (4)	C7—C8	1.521 (4)
O2—N1	1.182 (4)	C8—H8A	0.9700
N1—C1	1.479 (4)	C8—H8B	0.9700
C1—C2	1.374 (4)	C8—C9	1.505 (4)
C1—C6	1.373 (4)	C9—C10	1.384 (5)
C2—H2	0.9300	C9—C14	1.374 (4)
C2—C3	1.350 (5)	C10—H10	0.9300
C3—C4	1.348 (5)	C10—C11	1.378 (5)
C3—Cl1A	1.697 (9)	C11—H11	0.9300
C4—H4	0.9300	C11—C12	1.344 (5)
C4—C5	1.376 (5)	C12—H12	0.9300
C5—H5	0.9300	C12—C13	1.369 (5)
C5—C6	1.389 (5)	C13—H13	0.9300
C6—C7	1.502 (4)	C13—C14	1.386 (4)
C7—H7A	0.9700	C14—H14	0.9300
O1—N1—C1	120.1 (3)	C8—C7—H7A	109.0
O2—N1—O1	121.8 (4)	C8—C7—H7B	109.0
O2—N1—C1	118.1 (3)	C7—C8—H8A	109.2
C2—C1—N1	114.9 (3)	C7—C8—H8B	109.2
C6—C1—N1	121.5 (3)	H8A—C8—H8B	107.9
C6—C1—C2	123.6 (3)	C9—C8—C7	112.2 (3)
C1—C2—H2	120.3	C9—C8—H8A	109.2
C3—C2—C1	119.3 (3)	C9—C8—H8B	109.2
C3—C2—H2	120.3	C10—C9—C8	121.0 (3)
C2—C3—Cl1	115.1 (4)	C14—C9—C8	121.5 (3)
C2—C3—Cl1A	130.3 (12)	C14—C9—C10	117.5 (3)
C4—C3—Cl1	124.7 (4)	C9—C10—H10	119.6
C4—C3—C2	120.2 (3)	C11—C10—C9	120.7 (3)
C4—C3—Cl1A	109.4 (12)	C11—C10—H10	119.6
C3—C4—H4	120.1	C10—C11—H11	119.3
C3—C4—C5	119.8 (3)	C12—C11—C10	121.5 (4)
C5—C4—H4	120.1	C12—C11—H11	119.3
C4—C5—H5	118.7	C11—C12—H12	120.6
C4—C5—C6	122.6 (3)	C11—C12—C13	118.8 (3)

C6—C5—H5	118.7	C13—C12—H12	120.6
C1—C6—C5	114.5 (3)	C12—C13—H13	119.7
C1—C6—C7	127.9 (3)	C12—C13—C14	120.6 (4)
C5—C6—C7	117.6 (3)	C14—C13—H13	119.7
C6—C7—H7A	109.0	C9—C14—C13	120.8 (3)
C6—C7—H7B	109.0	C9—C14—H14	119.6
C6—C7—C8	112.9 (3)	C13—C14—H14	119.6
H7A—C7—H7B	107.8		

Cl1—C3—C4—C5	−178.1 (4)	C4—C5—C6—C1	1.0 (5)
O1—N1—C1—C2	172.2 (3)	C4—C5—C6—C7	−179.7 (3)
O1—N1—C1—C6	−9.1 (5)	C5—C6—C7—C8	−90.9 (4)
O2—N1—C1—C2	−6.8 (5)	C6—C1—C2—C3	1.2 (5)
O2—N1—C1—C6	171.9 (4)	C6—C7—C8—C9	−179.4 (3)
N1—C1—C2—C3	179.9 (3)	C7—C8—C9—C10	84.0 (4)
N1—C1—C6—C5	179.9 (3)	C7—C8—C9—C14	−93.4 (4)
N1—C1—C6—C7	0.7 (5)	C8—C9—C10—C11	−178.7 (3)
C1—C2—C3—Cl1	177.9 (3)	C8—C9—C14—C13	178.5 (3)
C1—C2—C3—C4	−0.4 (5)	C9—C10—C11—C12	1.0 (6)
C1—C2—C3—Cl1A	−176.5 (6)	C10—C9—C14—C13	1.0 (5)
C1—C6—C7—C8	88.3 (4)	C10—C11—C12—C13	−0.5 (6)
C2—C1—C6—C5	−1.4 (4)	C11—C12—C13—C14	0.3 (6)
C2—C1—C6—C7	179.3 (3)	C12—C13—C14—C9	−0.6 (5)
C2—C3—C4—C5	0.0 (6)	C14—C9—C10—C11	−1.2 (5)
C3—C4—C5—C6	−0.3 (6)	Cl1A—C3—C4—C5	176.8 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.54	3.462 (5)	175

Symmetry code: (i) *x*, −*y*+1/2, *z*+1/2.