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4-Chloro-1-[2-(2-chlorophenyl)ethyl]-2-nitrobenzene

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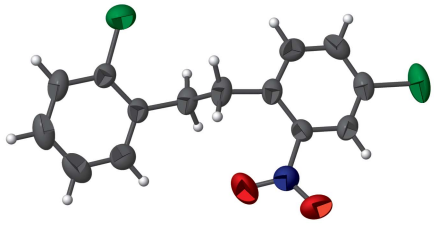
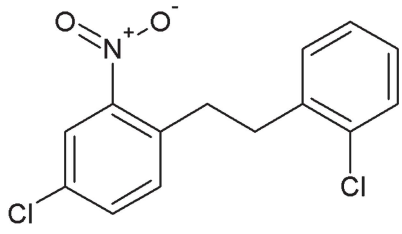
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{11}Cl_2NO_2$, the dihedral angle between the phenyl rings is 8.60 (17)° and the nitro group makes a dihedral anle of 29.4 (4)° with its attached ring. The crystal structure features C—H···O hydrogen bonds and π–π interactions.

3D view



Chemical scheme



Structure description

In continuation of our work on nitrobenzene derivatives, we report herein the crystal structure of the title compound (Anuradha *et al.*, 2014).

In the title compound (Fig. 1), the dihedral angle between the phenyl rings is 8.60 (17)° and the nitro group makes a dihedral anle of 29.4 (4)° with its attached ring. The crystal structure (Fig. 2 and Table 1) features infinite chains of C4—H···O1 hydrogen bonds along the *b* axis and weak π–π interactions ($Cg1\cdots Cg2^{i}$ = 3.672 (2) Å; *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 rings, respectively; symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$).

Synthesis and crystallization

The compound purchased from Sigma Aldrich and recrystallized from methanol solution.

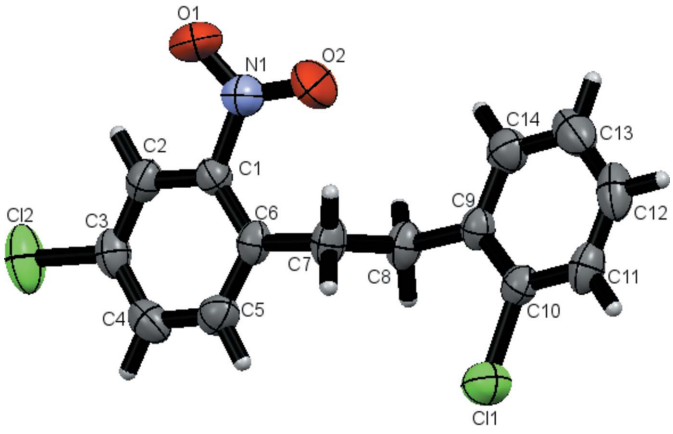


Figure 1
A view of the title molecule, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the DST–PURSE, Mangalore University, Mangaluru, for providing the single-crystal X-ray diffraction facility. PN and YHS acknowledge Bharthi College, Maddur, for research facilities.

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.60	3.335 (5)	137

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{11}Cl_2NO_2$
M_r	296.14
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	7.5774 (15), 13.244 (3), 13.488 (3)
β (°)	97.157 (7)
V (Å^3)	1343.0 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.48
Crystal size (mm)	0.3 × 0.23 × 0.12
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.874, 0.944
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8341, 2449, 1582
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.144, 1.04
No. of reflections	2449
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.44

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

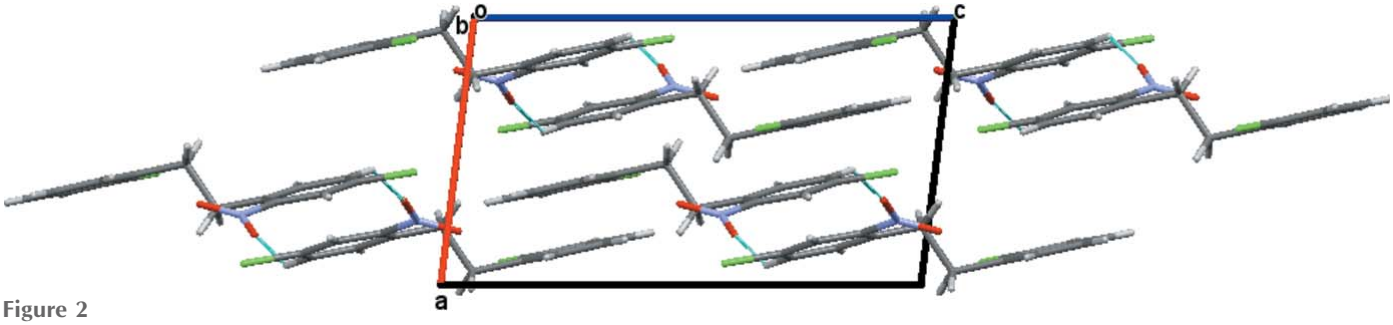

Figure 2
View along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are drawn as dashed lines.

full crystallographic data

IUCrData (2016). **1**, x161204 [https://doi.org/10.1107/S2414314616012049]

4-Chloro-1-[2-(2-chlorophenyl)ethyl]-2-nitrobenzene

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4-Chloro-1-[2-(2-chlorophenyl)ethyl]-2-nitrobenzene

Crystal data

$C_{14}H_{11}Cl_2NO_2$
M_r = 296.14
Monoclinic, $P2_1/n$
a = 7.5774 (15) Å
b = 13.244 (3) Å
c = 13.488 (3) Å
β = 97.157 (7)°
V = 1343.0 (5) Å^3
Z = 4
$F(000)$ = 608
D_x = 1.465 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 2449 reflections
θ = 3.0–25.3°
μ = 0.48 mm^{-1}
T = 293 K
Block, brown
0.3 × 0.23 × 0.12 mm

Data collection

Rigaku Saturn724+ diffractometer
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.874, T_{max} = 0.944
8341 measured reflections
2449 independent reflections
1582 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.4°, θ_{min} = 3.0°
h = −9→9
k = −15→15
l = −16→16
2449 standard reflections

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.144
S = 1.04
2449 reflections
172 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.8842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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}
Cl1	0.08248 (14)	0.02730 (7)	0.87941 (8)	0.0724 (4)
Cl2	0.07879 (15)	0.41848 (11)	1.41515 (7)	0.0874 (4)
O1	0.3135 (5)	0.5551 (2)	1.0990 (2)	0.0927 (10)
O2	0.1992 (5)	0.4658 (2)	0.9772 (2)	0.1112 (12)
N1	0.2398 (4)	0.4794 (2)	1.0660 (2)	0.0645 (9)
C1	0.1915 (4)	0.4026 (2)	1.1368 (2)	0.0431 (8)
C2	0.1617 (4)	0.4389 (3)	1.2292 (2)	0.0492 (8)
H2	0.1729	0.5075	1.2435	0.059*
C3	0.1157 (4)	0.3734 (3)	1.2988 (2)	0.0511 (9)
C4	0.1024 (5)	0.2721 (3)	1.2787 (3)	0.0578 (10)
H4	0.0714	0.2271	1.3265	0.069*
C5	0.1357 (5)	0.2381 (3)	1.1866 (3)	0.0542 (9)
H5	0.1274	0.1691	1.1740	0.065*
C6	0.1811 (4)	0.3011 (3)	1.1111 (2)	0.0444 (8)
C7	0.2166 (4)	0.2570 (3)	1.0130 (2)	0.0546 (9)
H7A	0.2666	0.1899	1.0243	0.066*
H7B	0.3037	0.2984	0.9850	0.066*
C8	0.0476 (4)	0.2502 (3)	0.9375 (2)	0.0527 (9)
H8A	−0.0301	0.1985	0.9590	0.063*
H8B	−0.0153	0.3141	0.9360	0.063*
C9	0.0892 (4)	0.2255 (3)	0.8342 (2)	0.0441 (8)
C10	0.1097 (4)	0.1285 (3)	0.8002 (2)	0.0463 (8)
C11	0.1495 (5)	0.1080 (3)	0.7050 (3)	0.0588 (10)
H11	0.1628	0.0415	0.6850	0.071*
C12	0.1691 (5)	0.1851 (4)	0.6406 (3)	0.0688 (12)
H12	0.1936	0.1717	0.5760	0.083*
C13	0.1521 (5)	0.2835 (4)	0.6720 (3)	0.0717 (12)
H13	0.1675	0.3367	0.6289	0.086*
C14	0.1126 (5)	0.3027 (3)	0.7667 (3)	0.0583 (10)
H14	0.1010	0.3694	0.7865	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0822 (7)	0.0552 (6)	0.0777 (7)	−0.0030 (5)	0.0022 (5)	0.0056 (5)
Cl2	0.0788 (7)	0.1404 (11)	0.0451 (5)	0.0111 (7)	0.0157 (5)	−0.0200 (6)
O1	0.138 (3)	0.0512 (17)	0.087 (2)	−0.0271 (19)	0.0045 (19)	0.0057 (15)
O2	0.181 (4)	0.105 (3)	0.0490 (18)	−0.049 (2)	0.020 (2)	0.0081 (17)
N1	0.084 (2)	0.054 (2)	0.056 (2)	−0.0080 (19)	0.0109 (17)	0.0006 (16)
C1	0.0464 (19)	0.0454 (19)	0.0375 (17)	0.0016 (16)	0.0053 (14)	0.0019 (15)
C2	0.051 (2)	0.0474 (19)	0.048 (2)	0.0021 (17)	−0.0005 (16)	−0.0103 (17)
C3	0.042 (2)	0.072 (3)	0.0390 (18)	0.0055 (18)	0.0051 (15)	−0.0066 (17)
C4	0.054 (2)	0.071 (3)	0.048 (2)	0.001 (2)	0.0039 (17)	0.0152 (19)
C5	0.056 (2)	0.044 (2)	0.060 (2)	0.0032 (18)	−0.0034 (18)	0.0009 (17)
C6	0.0382 (19)	0.052 (2)	0.0420 (18)	0.0050 (16)	0.0001 (14)	−0.0092 (16)

C7	0.050 (2)	0.063 (2)	0.049 (2)	0.0100 (19)	−0.0002 (17)	−0.0189 (17)
C8	0.048 (2)	0.060 (2)	0.048 (2)	0.0060 (18)	0.0025 (16)	−0.0140 (17)
C9	0.0397 (18)	0.050 (2)	0.0406 (18)	0.0051 (16)	−0.0029 (14)	−0.0055 (15)
C10	0.0419 (19)	0.048 (2)	0.0474 (19)	−0.0017 (16)	−0.0012 (15)	−0.0057 (15)
C11	0.055 (2)	0.070 (3)	0.052 (2)	0.001 (2)	0.0063 (17)	−0.024 (2)
C12	0.055 (2)	0.111 (4)	0.041 (2)	−0.010 (2)	0.0065 (17)	−0.014 (2)
C13	0.062 (3)	0.096 (3)	0.055 (2)	−0.017 (2)	−0.0012 (19)	0.018 (2)
C14	0.057 (2)	0.057 (2)	0.059 (2)	0.0012 (19)	−0.0039 (18)	0.0000 (19)

Geometric parameters (Å, º)

Cl1—C10	1.742 (4)	C7—H7B	0.9700
Cl2—C3	1.734 (3)	C7—C8	1.536 (4)
O1—N1	1.206 (4)	C8—H8A	0.9700
O2—N1	1.212 (4)	C8—H8B	0.9700
N1—C1	1.471 (4)	C8—C9	1.503 (4)
C1—C2	1.380 (4)	C9—C10	1.380 (4)
C1—C6	1.388 (4)	C9—C14	1.395 (5)
C2—H2	0.9300	C10—C11	1.381 (4)
C2—C3	1.356 (5)	C11—H11	0.9300
C3—C4	1.370 (5)	C11—C12	1.361 (5)
C4—H4	0.9300	C12—H12	0.9300
C4—C5	1.373 (5)	C12—C13	1.380 (6)
C5—H5	0.9300	C13—H13	0.9300
C5—C6	1.394 (5)	C13—C14	1.371 (5)
C6—C7	1.501 (4)	C14—H14	0.9300
C7—H7A	0.9700		

O1—N1—O2	122.4 (3)	C8—C7—H7B	109.1
O1—N1—C1	118.5 (3)	C7—C8—H8A	109.2
O2—N1—C1	119.1 (3)	C7—C8—H8B	109.2
C2—C1—N1	115.3 (3)	H8A—C8—H8B	107.9
C2—C1—C6	123.5 (3)	C9—C8—C7	111.9 (3)
C6—C1—N1	121.2 (3)	C9—C8—H8A	109.2
C1—C2—H2	120.4	C9—C8—H8B	109.2
C3—C2—C1	119.2 (3)	C10—C9—C8	123.8 (3)
C3—C2—H2	120.4	C10—C9—C14	115.9 (3)
C2—C3—Cl2	119.4 (3)	C14—C9—C8	120.3 (3)
C2—C3—C4	120.6 (3)	C9—C10—Cl1	119.1 (3)
C4—C3—Cl2	120.0 (3)	C9—C10—C11	122.6 (3)
C3—C4—H4	120.6	C11—C10—Cl1	118.4 (3)
C3—C4—C5	118.9 (3)	C10—C11—H11	120.0
C5—C4—H4	120.6	C12—C11—C10	120.0 (4)
C4—C5—H5	118.2	C12—C11—H11	120.0
C4—C5—C6	123.7 (3)	C11—C12—H12	120.3
C6—C5—H5	118.2	C11—C12—C13	119.4 (3)
C1—C6—C5	114.1 (3)	C13—C12—H12	120.3
C1—C6—C7	125.9 (3)	C12—C13—H13	120.0

C5—C6—C7	119.9 (3)	C14—C13—C12	120.0 (4)
C6—C7—H7A	109.1	C14—C13—H13	120.0
C6—C7—H7B	109.1	C9—C14—H14	118.9
C6—C7—C8	112.4 (3)	C13—C14—C9	122.1 (4)
H7A—C7—H7B	107.9	C13—C14—H14	118.9
C8—C7—H7A	109.1		

Cl1—C10—C11—C12	179.0 (3)	C4—C5—C6—C7	179.5 (3)
Cl2—C3—C4—C5	−178.7 (3)	C5—C6—C7—C8	89.9 (4)
O1—N1—C1—C2	27.5 (5)	C6—C1—C2—C3	−1.5 (5)
O1—N1—C1—C6	−151.4 (4)	C6—C7—C8—C9	168.7 (3)
O2—N1—C1—C2	−150.2 (4)	C7—C8—C9—C10	86.1 (4)
O2—N1—C1—C6	30.9 (5)	C7—C8—C9—C14	−92.7 (4)
N1—C1—C2—C3	179.7 (3)	C8—C9—C10—Cl1	1.2 (4)
N1—C1—C6—C5	179.4 (3)	C8—C9—C10—C11	−179.5 (3)
N1—C1—C6—C7	0.4 (5)	C8—C9—C14—C13	179.5 (3)
C1—C2—C3—Cl2	179.8 (2)	C9—C10—C11—C12	−0.3 (5)
C1—C2—C3—C4	1.3 (5)	C10—C9—C14—C13	0.5 (5)
C1—C6—C7—C8	−91.2 (4)	C10—C11—C12—C13	1.2 (6)
C2—C1—C6—C5	0.6 (5)	C11—C12—C13—C14	−1.2 (6)
C2—C1—C6—C7	−178.4 (3)	C12—C13—C14—C9	0.4 (6)
C2—C3—C4—C5	−0.3 (5)	C14—C9—C10—Cl1	−179.9 (2)
C3—C4—C5—C6	−0.6 (5)	C14—C9—C10—C11	−0.5 (5)
C4—C5—C6—C1	0.4 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.60	3.335 (5)	137
C7—H7*B*···O2	0.97	2.35	2.808 (5)	108
C8—H8*A*···Cl1	0.97	2.69	3.074 (4)	104

Symmetry code: (i) −*x*+1/2, *y*−1/2, −*z*+5/2.