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2,6-Dichloro-*N*-(4-methylphenyl)-benzamide

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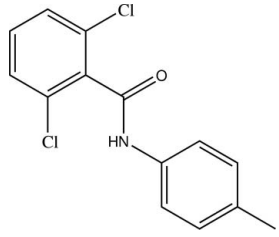
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.150; data-to-parameter ratio = 15.4.

In the title compound, $C_{14}H_{11}Cl_2NO$, the two benzene rings are non-coplanar [dihedral angle = 60.9 (3)°]. In the crystal, an amide N—H···O hydrogen bond links the molecules into chains which extend along (001).

Related literature

For the synthesis of the title compound, see: Houlihan *et al.* (1981). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{11}Cl_2NO$
M_r = 280.14
Monoclinic, $P2_1/c$
a = 11.260 (2) Å
b = 12.786 (3) Å
c = 9.6700 (19) Å
β = 100.65 (3)°
V = 1368.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 293 K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.874, T_{max} = 0.955
2650 measured reflections
2518 independent reflections
1514 reflections with $I > 2s(I)$
R_{int} = 0.033
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.150
S = 1.01
2518 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O^{i}	0.86	1.98	2.839 (4)	173

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank Liu Bo Nian from Nanjing University of Technology for useful discussions and the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2197).

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supplementary materials

Acta Cryst. (2012). E**68**, o1417 [doi:10.1107/S1600536812015188]

2,6-Dichloro-*N*-(4-methylphenyl)benzamide

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Comment

We report here the crystal structure of the title compound $C_{14}H_{11}Cl_2NO$. In this molecule (Fig. 1), the phenyl and dichlorophenyl rings are non-coplanar [dihedral angle 60.9 (3)°]. In the crystal structure an intermolecular amide N—H···O hydrogen bond (Table 1) links the molecules, giving one-dimensional chains which extend along (001) (Fig. 2).

Experimental

A mixture of 4-methylbenzenamine (3.2 g, 0.03 mol), 2,6-dichlorobenzoyl chloride (6.3 g, 0.03 mol), and 6 ml of triethylamine in 50 ml of anhydrous tetrahydrofuran was refluxed with stirring for 8 h and then allowed to stand at room temperature. The resulting solids were filtered off and washed with water (2 x 30 mL) then dried, giving 7.2 g of product. Recrystallization from ethanol gave yellow crystals of the title compound. Crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

Hydrogen atoms were positioned geometrically, with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl) and N—H = 0.86 Å and were allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(aromatic C, N) or 1.5U_{eq}(methyl C).

Computing details

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software* (Enraf–Nonius, 1989); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

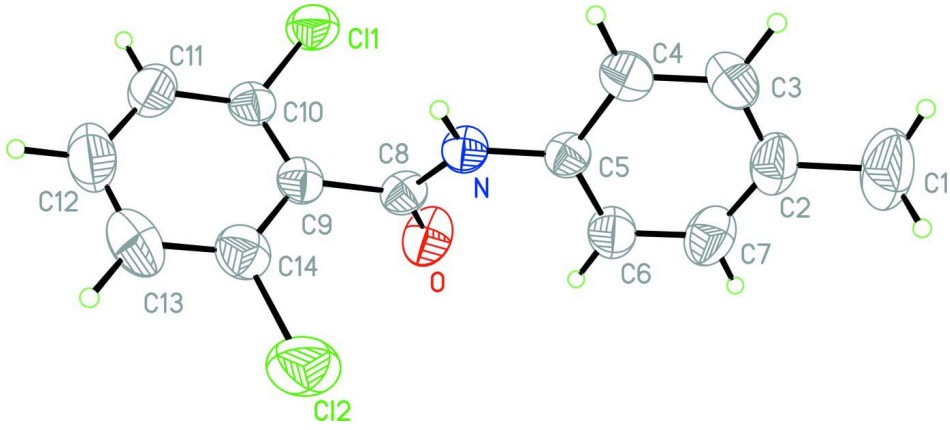

Figure 1

The molecular structure of the title compound showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level.

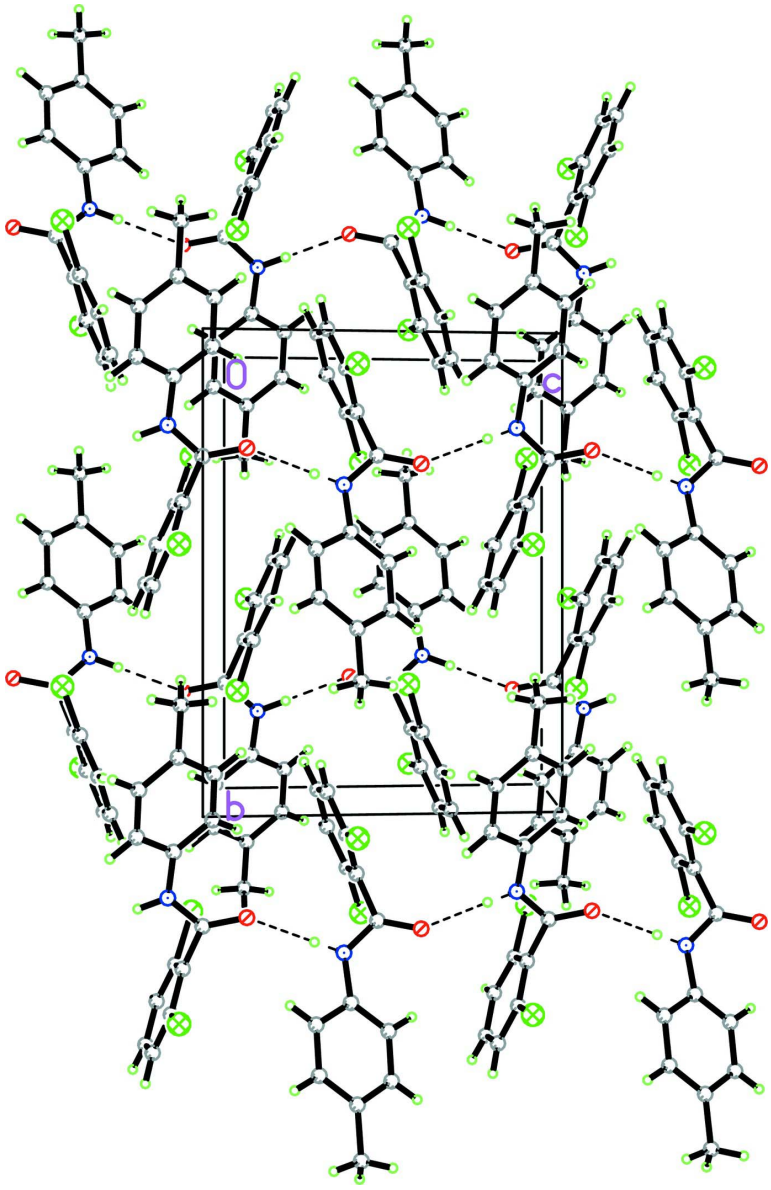

Figure 2

A packing diagram of the title compound viewed down *a*, with intermolecular hydrogen bonds shown as dashed lines.

2,6-Dichloro-*N*-(4-methylphenyl)benzamide

Crystal data

$C_{14}H_{11}Cl_2NO$
$M_r = 280.14$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.260$ (2) Å
$b = 12.786$ (3) Å
$c = 9.6700$ (19) Å
$\beta = 100.65$ (3)°
$V = 1368.2$ (5) Å^3
$Z = 4$

$F(000) = 576$
$D_x = 1.360$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–13°
$\mu = 0.46$ mm^{-1}
$T = 293$ K
Block, yellow
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.874, T_{max} = 0.955
2650 measured reflections
2518 independent reflections
1514 reflections with $I > 2s\breve{}I$)
R_{int} = 0.033
θ_{max} = 25.4°, θ_{min} = 1.8°
$h = -13\rightarrow0$
$k = 0\rightarrow15$
$l = -11\rightarrow11$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.150
S = 1.01
2518 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) 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}
N	0.2641 (2)	0.8121 (2)	0.1158 (3)	0.0404 (7)
H0A	0.2757	0.7889	0.2007	0.048*
O	0.2803 (3)	0.76570 (19)	−0.1064 (2)	0.0660 (8)
Cl1	0.14387 (9)	0.55959 (8)	0.07524 (10)	0.0635 (3)
C1	0.0707 (4)	1.2269 (3)	0.0646 (6)	0.0969 (17)
H1A	0.0283	1.2398	0.1404	0.145*
H1B	0.0162	1.2352	−0.0236	0.145*
H1C	0.1361	1.2758	0.0699	0.145*
Cl2	0.56778 (10)	0.75531 (9)	0.07081 (15)	0.0876 (4)
C2	0.1203 (3)	1.1167 (3)	0.0760 (5)	0.0601 (11)
C3	0.1026 (4)	1.0507 (3)	0.1828 (4)	0.0629 (11)
H3A	0.0596	1.0745	0.2500	0.076*
C4	0.1474 (3)	0.9499 (3)	0.1924 (4)	0.0533 (9)
H4A	0.1334	0.9065	0.2649	0.064*
C5	0.2128 (3)	0.9131 (2)	0.0952 (3)	0.0395 (8)
C6	0.2314 (3)	0.9779 (3)	−0.0124 (4)	0.0562 (10)

H6A	0.2750	0.9544	−0.0791	0.067*
C7	0.1848 (4)	1.0781 (3)	−0.0206 (4)	0.0661 (11)
H7A	0.1975	1.1210	−0.0941	0.079*
C8	0.2970 (3)	0.7476 (3)	0.0202 (3)	0.0423 (8)
C9	0.3616 (3)	0.6510 (3)	0.0813 (3)	0.0418 (8)
C10	0.3010 (3)	0.5611 (3)	0.1098 (3)	0.0445 (8)
C11	0.3614 (4)	0.4729 (3)	0.1667 (4)	0.0592 (10)
H11A	0.3192	0.4132	0.1837	0.071*
C12	0.4849 (4)	0.4751 (4)	0.1976 (5)	0.0730 (13)
H12A	0.5265	0.4165	0.2380	0.088*
C13	0.5485 (4)	0.5612 (4)	0.1707 (4)	0.0710 (12)
H13A	0.6324	0.5614	0.1921	0.085*
C14	0.4868 (3)	0.6472 (3)	0.1116 (4)	0.0550 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.0548 (17)	0.0427 (16)	0.0246 (13)	0.0042 (13)	0.0096 (12)	0.0009 (12)
O	0.112 (2)	0.0577 (16)	0.0291 (13)	0.0081 (15)	0.0157 (13)	−0.0012 (12)
Cl1	0.0531 (6)	0.0723 (7)	0.0669 (7)	−0.0039 (5)	0.0156 (5)	0.0100 (5)
C1	0.092 (4)	0.054 (3)	0.139 (5)	0.020 (3)	0.007 (3)	0.002 (3)
Cl2	0.0715 (8)	0.0718 (8)	0.1247 (11)	−0.0208 (6)	0.0314 (7)	−0.0195 (7)
C2	0.049 (2)	0.044 (2)	0.082 (3)	0.0040 (18)	0.000 (2)	−0.003 (2)
C3	0.062 (3)	0.060 (3)	0.072 (3)	0.008 (2)	0.027 (2)	−0.010 (2)
C4	0.060 (2)	0.054 (2)	0.050 (2)	0.0024 (19)	0.0204 (18)	−0.0009 (18)
C5	0.0430 (18)	0.0413 (19)	0.0337 (17)	−0.0001 (15)	0.0059 (14)	0.0015 (15)
C6	0.074 (3)	0.052 (2)	0.047 (2)	0.009 (2)	0.0222 (19)	0.0045 (18)
C7	0.083 (3)	0.051 (2)	0.063 (3)	0.003 (2)	0.010 (2)	0.013 (2)
C8	0.051 (2)	0.0449 (19)	0.0318 (18)	−0.0029 (16)	0.0087 (15)	0.0000 (16)
C9	0.050 (2)	0.045 (2)	0.0323 (17)	0.0039 (16)	0.0115 (15)	−0.0071 (15)
C10	0.050 (2)	0.051 (2)	0.0338 (17)	0.0035 (18)	0.0131 (15)	−0.0029 (17)
C11	0.072 (3)	0.051 (2)	0.057 (2)	0.008 (2)	0.018 (2)	0.0078 (18)
C12	0.073 (3)	0.067 (3)	0.077 (3)	0.027 (3)	0.011 (2)	0.009 (2)
C13	0.048 (2)	0.086 (3)	0.076 (3)	0.016 (2)	0.002 (2)	−0.004 (3)
C14	0.054 (2)	0.053 (2)	0.060 (2)	−0.0002 (19)	0.0143 (18)	−0.0102 (19)

Geometric parameters (Å, º)

N—C8	1.341 (4)	C4—H4A	0.9300
N—C5	1.414 (4)	C5—C6	1.376 (4)
N—H0A	0.8600	C6—C7	1.381 (5)
O—C8	1.225 (4)	C6—H6A	0.9300
Cl1—C10	1.739 (4)	C7—H7A	0.9300
C1—C2	1.513 (5)	C8—C9	1.498 (5)
C1—H1A	0.9600	C9—C14	1.387 (5)
C1—H1B	0.9600	C9—C10	1.390 (5)
C1—H1C	0.9600	C10—C11	1.379 (5)
Cl2—C14	1.740 (4)	C11—C12	1.367 (6)
C2—C7	1.376 (5)	C11—H11A	0.9300
C2—C3	1.377 (5)	C12—C13	1.365 (6)

C3—C4	1.381 (5)	C12—H12A	0.9300
C3—H3A	0.9300	C13—C14	1.368 (5)
C4—C5	1.379 (4)	C13—H13A	0.9300
C8—N—C5	128.5 (3)	C2—C7—C6	122.4 (4)
C8—N—H0A	115.8	C2—C7—H7A	118.8
C5—N—H0A	115.8	C6—C7—H7A	118.8
C2—C1—H1A	109.5	O—C8—N	124.2 (3)
C2—C1—H1B	109.5	O—C8—C9	121.6 (3)
H1A—C1—H1B	109.5	N—C8—C9	114.2 (3)
C2—C1—H1C	109.5	C14—C9—C10	116.5 (3)
H1A—C1—H1C	109.5	C14—C9—C8	120.8 (3)
H1B—C1—H1C	109.5	C10—C9—C8	122.7 (3)
C7—C2—C3	117.2 (4)	C11—C10—C9	122.1 (3)
C7—C2—C1	121.3 (4)	C11—C10—Cl1	118.5 (3)
C3—C2—C1	121.5 (4)	C9—C10—Cl1	119.4 (3)
C2—C3—C4	121.4 (4)	C12—C11—C10	118.5 (4)
C2—C3—H3A	119.3	C12—C11—H11A	120.7
C4—C3—H3A	119.3	C10—C11—H11A	120.7
C5—C4—C3	120.5 (3)	C13—C12—C11	121.5 (4)
C5—C4—H4A	119.8	C13—C12—H12A	119.2
C3—C4—H4A	119.8	C11—C12—H12A	119.2
C6—C5—C4	119.0 (3)	C12—C13—C14	119.0 (4)
C6—C5—N	122.8 (3)	C12—C13—H13A	120.5
C4—C5—N	118.1 (3)	C14—C13—H13A	120.5
C5—C6—C7	119.5 (3)	C13—C14—C9	122.3 (4)
C5—C6—H6A	120.2	C13—C14—Cl2	119.1 (3)
C7—C6—H6A	120.2	C9—C14—Cl2	118.6 (3)
C7—C2—C3—C4	−0.2 (6)	O—C8—C9—C10	−96.5 (4)
C1—C2—C3—C4	179.6 (4)	N—C8—C9—C10	85.6 (4)
C2—C3—C4—C5	0.8 (6)	C14—C9—C10—C11	0.7 (5)
C3—C4—C5—C6	−0.8 (5)	C8—C9—C10—C11	−179.7 (3)
C3—C4—C5—N	175.4 (3)	C14—C9—C10—Cl1	179.8 (2)
C8—N—C5—C6	−26.7 (5)	C8—C9—C10—Cl1	−0.5 (4)
C8—N—C5—C4	157.2 (3)	C9—C10—C11—C12	1.0 (5)
C4—C5—C6—C7	0.2 (5)	Cl1—C10—C11—C12	−178.2 (3)
N—C5—C6—C7	−175.8 (3)	C10—C11—C12—C13	−1.4 (6)
C3—C2—C7—C6	−0.4 (6)	C11—C12—C13—C14	0.2 (7)
C1—C2—C7—C6	179.8 (4)	C12—C13—C14—C9	1.6 (6)
C5—C6—C7—C2	0.4 (6)	C12—C13—C14—Cl2	−177.5 (3)
C5—N—C8—O	−4.5 (5)	C10—C9—C14—C13	−2.0 (5)
C5—N—C8—C9	173.4 (3)	C8—C9—C14—C13	178.4 (3)
O—C8—C9—C14	83.1 (4)	C10—C9—C14—Cl2	177.1 (2)
N—C8—C9—C14	−94.8 (4)	C8—C9—C14—Cl2	−2.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0*A*···O^{i}	0.86	1.98	2.839 (4)	173

Symmetry code: (i) *x*, −*y*+3/2, *z*+1/2.