2,2-Dichloro-*N*-(3,5-dimethylphenyl)-acetamide

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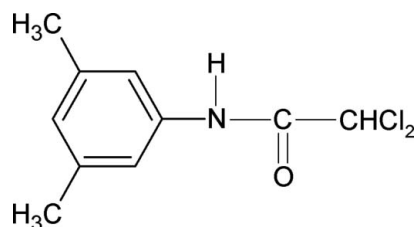
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The structure of the title compound, $C_{10}H_{11}Cl_2NO$, resembles those of 2,2-dichloro-*N*-phenylacetamide, 2,2-dichloro-*N*-(2-methylphenyl)acetamide, 2,2-dichloro-*N*-(3-methylphenyl)-acetamide, 2,2-dichloro-*N*-(4-methylphenyl)acetamide, *N*-(3,5-dimethylphenyl)acetamide and other acetanilides, with similar bond parameters. The molecules in the title compound are linked into infinite chains through N—H···O and C—H···O hydrogen bonding.

Related literature

For related literature, see: Gowda *et al.* (2001, 2006, 2007); Shilpa & Gowda (2007).

Experimental

Crystal data

$C_{10}H_{11}Cl_2NO$	$c = 9.163$ (3) Å
$M_r = 232.10$	$\beta = 110.99$ (2)°
Monoclinic, $P2_1/c$	$V = 1031.9$ (6) Å^3
$a = 11.412$ (4) Å	$Z = 4$
$b = 10.570$ (4) Å	Mo $K\alpha$ radiation
$\mu = 0.59$ mm^{-1}	$0.80 \times 0.26 \times 0.13$ mm
$T = 297$ (2) K	

Data collection

Stoe STADI-4 four-circle diffractometer	1825 independent reflections
Absorption correction: ψ-sacn (North *et al.*, 1968)	1445 reflections with $I > 2\sigma(I)$
$T_{min} = 0.873$, $T_{max} = 0.927$	3 standard reflections frequency: 120 min intensity decay: 1%
1825 measured reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.179$	
$S = 1.07$	
1825 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
133 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6N···O5[i]	0.78 (4)	2.12 (4)	2.857 (4)	159 (4)
C3—H3···O5[i]	0.98	2.38	3.252 (4)	148

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

Data collection: *STADI4* (Stoe & Cie, 1987); cell refinement: *STADI4*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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supporting information

2,2-Dichloro-*N*-(3,5-dimethylphenyl)acetamide

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S1. Comment

In the present work, the structure of 2,2-dichloro-*N*- (3,5-dimethylphenyl)-acetamide (35DMPDCA) has been determined to explore the substituent effects on the structures of *N*-aromatic amides (Gowda *et al.*, 2001, 2006, 2007). The structure of 35DMPDCA (Fig. 1) resembles those of 2,2-dichloro-*N*-(phenyl)acetamide (PDCA)(Gowda *et al.*, 2001), 2,2-di-chloro-*N*-(2-methylphenyl)acetamide (2MPDCA)(Gowda *et al.*, 2006), 2,2-dichloro-*N*-(3-methylphenyl)-acetamide (3MPDCA) (Gowda *et al.*, 2006), 2,2-dichloro-*N*-(4-methylphenyl)-acetamide (4MPDCA)(Gowda *et al.*, 2001) and *N*-(3,5-dimethylphenyl)-acetamide (35DMPA)(Gowda *et al.*, 2007). But the 35DMPDCA has a single molecule in its asymmetric unit, in contrast to two molecules observed in the asymmetric unit of 35DMPA. The bond parameters in 35DMPDCA are similar to those in PDCA, 2MPDCA, 3MPDCA, 4MPDCA, 35DMPA and other acetanilides (Gowda *et al.*, 2001, 2006; 2007). The molecules in 35DMPDcA are linked into zigzag chains through N—H⋯O and C—H⋯O hydrogen bonding (Table 1 and Fig.2).

S2. Experimental

The title compound was prepared according to the literature method (Shilpa and Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Shilpa and Gowda, 2007). Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH$_3$) or 0.98 Å (CHCl$_2$) with $U_{iso}(H) = 1.2 U_{eq}(CH)$ and $U_{iso}(H) = 1.4 U_{eq}(CH_3)$.
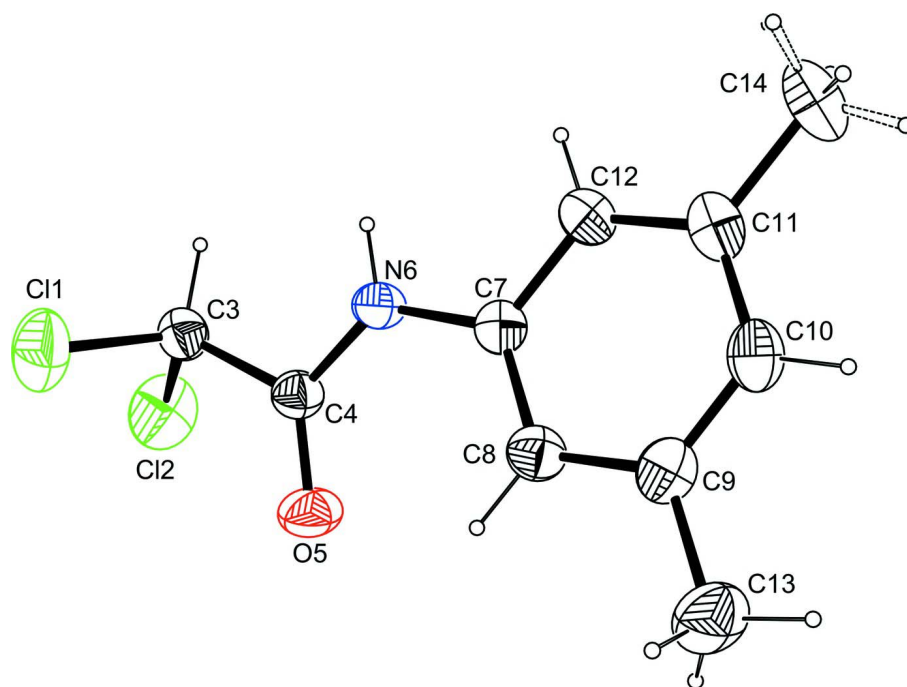
Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.
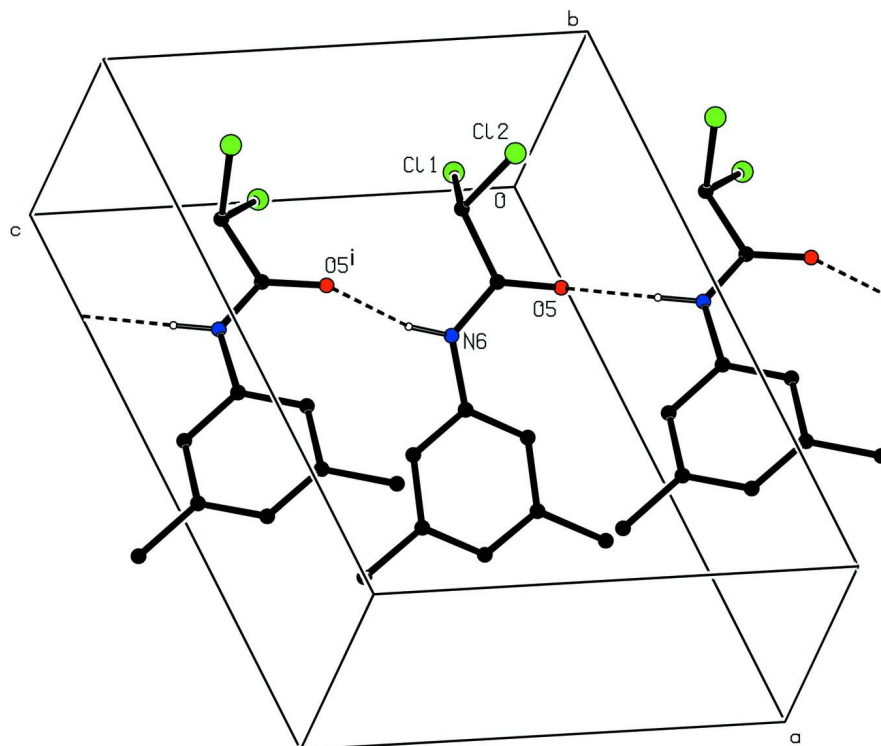
Figure 2

Partial packing view showing the formation of the chain through N—H···O hydrogen bondings. H atoms not involved in H bonds have been omitted for clarity. H bonds are shown as dashed lines. [Symmetry code: (i) x, $-y + 1/2$, $z + 1/2$]

2,2-Dichloro-*N*-(3,5-dimethylphenyl)acetamide

Crystal data

$C_{10}H_{11}Cl_2NO$	$F(000) = 480$
$M_r = 232.10$	$D_x = 1.494$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 44 reflections
$a = 11.412$ (4) Å	$\theta = 17.6–19.7°$
$b = 10.570$ (4) Å	$\mu = 0.59$ mm^{-1}
$c = 9.163$ (3) Å	$T = 297$ K
$\beta = 110.99$ (2)°	Prism, light yellow
$V = 1031.9$ (6) Å^3	$0.80 \times 0.26 \times 0.13$ mm
$Z = 4$	

Data collection

Stoe STADI-4 four-circle diffractometer	1825 independent reflections
Radiation source: fine-focus sealed tube	1445 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.000$
Profile fitted scans $2\theta/\omega=1/1$	$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
Absorption correction: numerical (North *et al.*, 1968)	$h = -13 \rightarrow 12$
	$k = 0 \rightarrow 12$
	$l = 0 \rightarrow 10$
$T_{min} = 0.873$, $T_{max} = 0.927$	3 standard reflections every 120 min
1825 measured reflections	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.059$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.179$	
$S = 1.07$	H atoms treated by a mixture of independent and constrained refinement
1825 reflections	
133 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.8161P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} = 0.015$
	$\Delta\rho_{max} = 0.62$ e Å^{-3}
	$\Delta\rho_{min} = -0.49$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
Cl1	−0.00025 (11)	0.11758 (11)	0.14291 (16)	0.0946 (5)	
Cl2	0.03634 (11)	0.35402 (11)	0.07162 (15)	0.0921 (5)	
C3	0.0997 (3)	0.2384 (3)	0.2002 (4)	0.0532 (8)	
H3	0.1084	0.2653	0.3059	0.064*	
C4	0.2273 (3)	0.2054 (3)	0.1930 (3)	0.0471 (7)	
O5	0.2424 (2)	0.1976 (3)	0.0688 (2)	0.0668 (7)	
N6	0.3146 (2)	0.1846 (2)	0.3333 (3)	0.0460 (6)	
H6N	0.300 (3)	0.199 (3)	0.408 (4)	0.055*	
C7	0.4409 (3)	0.1498 (3)	0.3696 (3)	0.0442 (7)	
C8	0.4852 (3)	0.1039 (3)	0.2593 (4)	0.0522 (8)	
H8	0.4318	0.0955	0.1558	0.063*	
C9	0.6106 (3)	0.0702 (3)	0.3040 (4)	0.0580 (8)	
C10	0.6875 (3)	0.0818 (3)	0.4575 (4)	0.0602 (9)	
H10	0.7713	0.0583	0.4866	0.072*	
C11	0.6444 (3)	0.1270 (3)	0.5694 (4)	0.0574 (8)	
C12	0.5203 (3)	0.1600 (3)	0.5236 (4)	0.0511 (8)	
H12	0.4889	0.1899	0.5977	0.061*	
C13	0.6583 (4)	0.0221 (5)	0.1825 (5)	0.0855 (13)	
H13A	0.6346	0.0795	0.0956	0.120*	
H13B	0.6229	−0.0598	0.1476	0.120*	
H13C	0.7481	0.0155	0.2262	0.120*	
C14	0.7311 (4)	0.1379 (4)	0.7388 (5)	0.0799 (12)	
H14A	0.8149	0.1555	0.7434	0.112*	0.46 (5)
H14B	0.7304	0.0598	0.7920	0.112*	0.46 (5)

H14C	0.7029	0.2053	0.7883	0.112*	0.46 (5)
H14D	0.6839	0.1250	0.8057	0.112*	0.54 (5)
H14E	0.7684	0.2206	0.7571	0.112*	0.54 (5)
H14F	0.7959	0.0751	0.7609	0.112*	0.54 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0748 (8)	0.0835 (8)	0.1257 (11)	−0.0243 (5)	0.0362 (7)	−0.0154 (6)
Cl2	0.0778 (8)	0.0821 (8)	0.1134 (9)	0.0310 (6)	0.0306 (6)	0.0280 (6)
C3	0.0472 (16)	0.0593 (19)	0.0507 (16)	0.0001 (14)	0.0146 (13)	−0.0023 (14)
C4	0.0502 (17)	0.0486 (16)	0.0425 (15)	0.0020 (13)	0.0165 (13)	0.0035 (12)
O5	0.0634 (15)	0.0949 (19)	0.0436 (12)	0.0195 (13)	0.0211 (10)	0.0148 (12)
N6	0.0494 (14)	0.0508 (14)	0.0388 (13)	0.0056 (11)	0.0171 (11)	0.0011 (11)
C7	0.0463 (16)	0.0370 (14)	0.0482 (16)	0.0021 (11)	0.0156 (13)	0.0052 (11)
C8	0.0566 (19)	0.0501 (16)	0.0490 (16)	0.0047 (14)	0.0176 (14)	0.0033 (13)
C9	0.0567 (19)	0.0496 (17)	0.070 (2)	0.0057 (14)	0.0258 (17)	0.0038 (15)
C10	0.0480 (18)	0.0505 (17)	0.076 (2)	0.0062 (14)	0.0153 (16)	0.0040 (16)
C11	0.0530 (19)	0.0431 (16)	0.065 (2)	−0.0012 (13)	0.0074 (16)	0.0028 (14)
C12	0.0547 (19)	0.0457 (16)	0.0479 (16)	0.0013 (14)	0.0123 (14)	−0.0001 (13)
C13	0.080 (3)	0.096 (3)	0.089 (3)	0.027 (2)	0.041 (2)	−0.001 (2)
C14	0.065 (2)	0.072 (2)	0.074 (2)	0.0028 (19)	−0.0092 (19)	−0.0078 (19)

Geometric parameters (Å, º)

Cl1—C3	1.667 (3)	C10—C11	1.372 (5)
Cl2—C3	1.671 (3)	C10—H10	0.9300
C3—C4	1.522 (4)	C11—C12	1.371 (5)
C3—H3	0.9800	C11—C14	1.518 (5)
C4—O5	1.213 (4)	C12—H12	0.9300
C4—N6	1.333 (4)	C13—H13A	0.9600
N6—C7	1.407 (4)	C13—H13B	0.9600
N6—H6N	0.78 (4)	C13—H13C	0.9600
C7—C8	1.370 (4)	C14—H14A	0.9600
C7—C12	1.381 (4)	C14—H14B	0.9600
C8—C9	1.387 (5)	C14—H14C	0.9600
C8—H8	0.9300	C14—H14D	0.9600
C9—C10	1.370 (5)	C14—H14E	0.9600
C9—C13	1.493 (5)	C14—H14F	0.9600
C4—C3—Cl1	111.6 (2)	C7—C12—H12	119.3
C4—C3—Cl2	108.4 (2)	C9—C13—H13A	109.5
Cl1—C3—Cl2	105.31 (18)	C9—C13—H13B	109.5
C4—C3—H3	110.5	H13A—C13—H13B	109.5
Cl1—C3—H3	110.5	C9—C13—H13C	109.5
Cl2—C3—H3	110.5	H13A—C13—H13C	109.5
O5—C4—N6	125.8 (3)	H13B—C13—H13C	109.5
O5—C4—C3	121.0 (3)	C11—C14—H14A	109.5

N6—C4—C3	113.1 (3)	C11—C14—H14B	109.5
C4—N6—C7	128.3 (3)	H14A—C14—H14B	109.5
C4—N6—H6N	120 (3)	C11—C14—H14C	109.5
C7—N6—H6N	112 (3)	H14A—C14—H14C	109.5
C8—C7—C12	120.1 (3)	H14B—C14—H14C	109.5
C8—C7—N6	122.4 (3)	C11—C14—H14D	109.5
C12—C7—N6	117.6 (3)	H14A—C14—H14D	141.1
C7—C8—C9	119.2 (3)	H14B—C14—H14D	56.3
C7—C8—H8	120.4	H14C—C14—H14D	56.3
C9—C8—H8	120.4	C11—C14—H14E	109.5
C10—C9—C8	119.6 (3)	H14A—C14—H14E	56.3
C10—C9—C13	121.7 (3)	H14B—C14—H14E	141.1
C8—C9—C13	118.7 (3)	H14C—C14—H14E	56.3
C9—C10—C11	121.9 (3)	H14D—C14—H14E	109.5
C9—C10—H10	119.0	C11—C14—H14F	109.5
C11—C10—H10	119.0	H14A—C14—H14F	56.3
C12—C11—C10	117.9 (3)	H14B—C14—H14F	56.3
C12—C11—C14	121.2 (4)	H14C—C14—H14F	141.1
C10—C11—C14	121.0 (3)	H14D—C14—H14F	109.5
C11—C12—C7	121.4 (3)	H14E—C14—H14F	109.5
C11—C12—H12	119.3		
Cl1—C3—C4—O5	73.5 (4)	C7—C8—C9—C10	0.8 (5)
Cl2—C3—C4—O5	−42.1 (4)	C7—C8—C9—C13	−179.2 (3)
Cl1—C3—C4—N6	−105.2 (3)	C8—C9—C10—C11	−0.6 (5)
Cl2—C3—C4—N6	139.3 (2)	C13—C9—C10—C11	179.4 (4)
O5—C4—N6—C7	0.0 (5)	C9—C10—C11—C12	0.5 (5)
C3—C4—N6—C7	178.5 (3)	C9—C10—C11—C14	179.5 (3)
C4—N6—C7—C8	−15.4 (5)	C10—C11—C12—C7	−0.8 (5)
C4—N6—C7—C12	166.3 (3)	C14—C11—C12—C7	−179.8 (3)
C12—C7—C8—C9	−1.1 (5)	C8—C7—C12—C11	1.1 (5)
N6—C7—C8—C9	−179.3 (3)	N6—C7—C12—C11	179.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*N*···O5[i]	0.78 (4)	2.12 (4)	2.857 (4)	159 (4)
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