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2-Chloro-*N*-(2,6-dimethylphenyl)-acetamide

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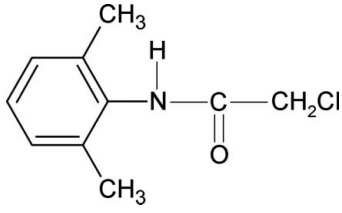
Key indicators: single-crystal X-ray study; T = 300 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.104; data-to-parameter ratio = 9.7.

The crystal structure of the title compound (26DMPCA), $C_{10}H_{12}ClNO$, is closely related to those of side-chain-unsubstituted *N*-(2,6-dimethylphenyl)acetamide and side-chain-substituted 2,2,2-trichloro-*N*-(2,6-dimethylphenyl)acetamide and *N*-(2,6-dimethylphenyl)-2,2,2-trimethylacetamide, with slightly different bond parameters. The molecules in 26DMPCA are linked into chains through N—H···O hydrogen bonding.

Related literature

For related literature, see: Gowda *et al.* (2004, 2007*a*,*b*,*c*,*d*,*e*,*f*); Gowda, Kozisek *et al.* (2007); Gowda, Svoboda & Fuess (2007).



Experimental

Crystal data

$C_{10}H_{12}ClNO$
M_r = 197.66
Monoclinic, $P2_1/c$
a = 13.766 (3) Å
b = 8.911 (2) Å
c = 8.538 (2) Å
β = 99.00 (1)°
V = 1034.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 300 (2) K
0.50 × 0.15 × 0.12 mm

Data collection

Stoe Stadi-4 diffractometer
Absorption correction: numerical (North *et al.*, 1968)
T_{min} = 0.952, T_{max} = 0.968
1318 measured reflections
1188 independent reflections
1053 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 22.5°
3 standard reflections
frequency: 200 min
intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
S = 1.10
1188 reflections
123 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···O4^{i}	0.86 (3)	2.04 (3)	2.866 (3)	161 (3)

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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2052).

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supporting information

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2-Chloro-*N*-(2,6-dimethylphenyl)acetamide

B. Thimme Gowda, Sabine Foro, Ingrid Svoboda, Helmut Paulus and Hartmut Fuess

S1. Comment

In the present work, the structure of 2-chloro-*N*-(2,6-dimethylphenyl)- acetamide (26DMPCA) has been determined as part of a study of the effect of ring and side chain substitutions on the solid state geometry of chemically and biologically significant compounds such as acetanilides (Gowda *et al.*, 2007*a*, 2007*b*, 2007*c*, 2007*d*, 2007*e*). The structure of 26DMPCA is closely related to the side chain unsubstituted *N*-(2,6-dimethylphenyl)-acetamide (26DMPA) (Gowda *et al.*, 2007*c*) and side chain substituted, 2,2,2-trichloro-*N*-(2,6-dimethylphenyl)-acetamide (26DMPTCA) (Gowda *et al.*, 2007*b*) and 2,2,2-trimethyl-*N*- (2,6-dimethylphenyl)-acetamide (26DMPTMA) (Gowda *et al.*, 2007*d*). The bond parameters in 26DMPCA are similar to those in 26DMPA, 26DMPTCA, 26DMPTMA and other acetanilides (Gowda *et al.*, 2007*a*, 2007*b*, 2007*c*, 2007*d*, 2007*e*). The molecules in 26DMPcA are linked into infinite chains through N—H···O hydrogen bonding (Table 1 and Fig.2).

S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2004). The purity of the compound was checked by determining its melting point. The compound was further characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2004). Single crystals of the title compound were obtained from a slow evaporation of 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 0.97 Å (CH_2Cl) and N—H = 0.86 Å with U_{iso}(H) = 1.2 U_{eq}(CH or NH) and U_{iso}(H) = 1.4 U_{eq}(CH_3).

Since the compound was prepared in a project that ended a few years ago, the measurement was performed using the theta range that was routinely applied at that time. In view of the fact that the structure is an organic compound, which scatters with minor intensity at high theta values we feel that the presented structural information on this compound is reliable enough in order to unambigiously solve the structure and refine the structure model reliably.

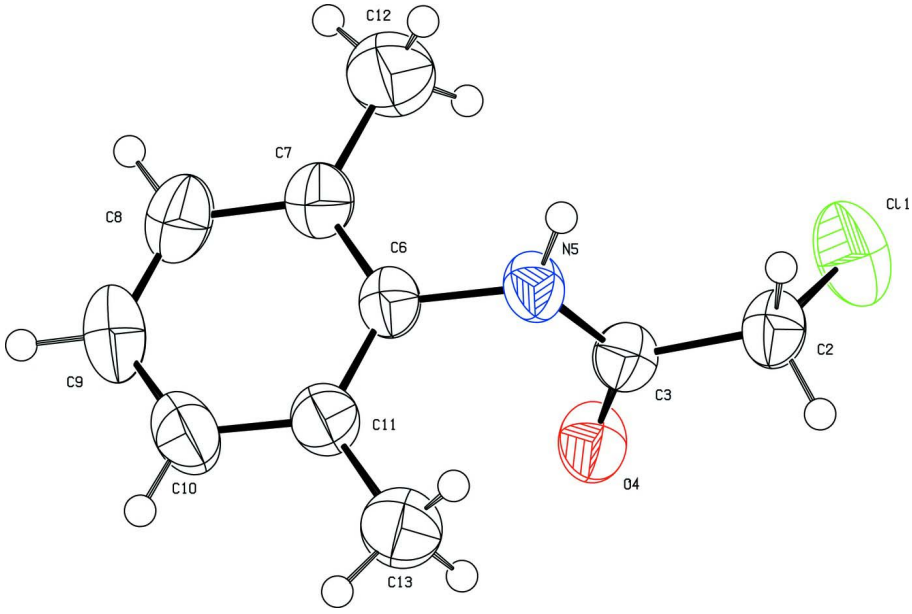

Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

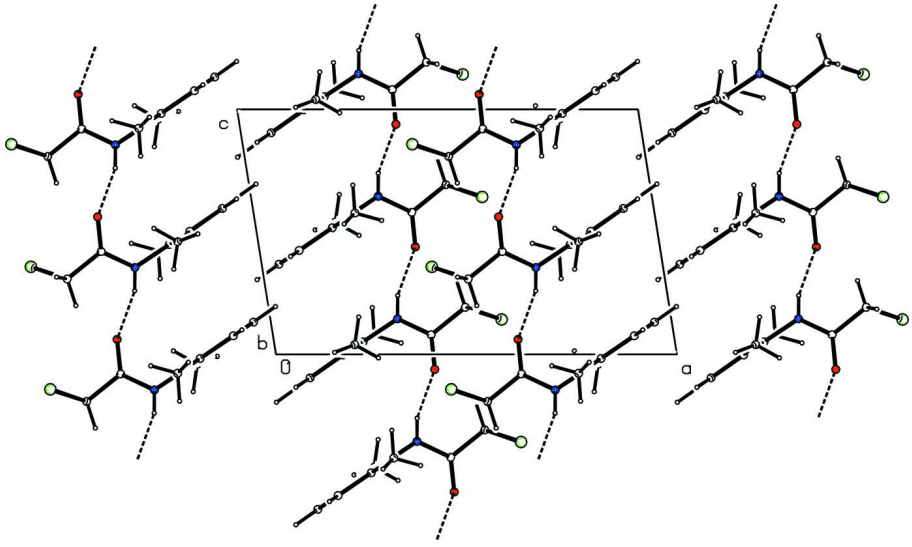

Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

2-Chloro-*N*-(2,6-dimethylphenyl)acetamide

Crystal data

$C_{10}H_{12}ClNO$
$M_r = 197.66$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.766\ (3)$ Å
$b = 8.911\ (2)$ Å
$c = 8.538\ (2)$ Å
$\beta = 99.00\ (1)°$
$V = 1034.4\ (4)$ Å^3
$Z = 4$
$F(000) = 416$
$D_x = 1.269$ Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 40 reflections
θ = 18.0–20.9°
μ = 0.33 mm^{-1}
T = 300 K
Needle, colourless
0.50 × 0.15 × 0.12 mm

Data collection

Stoe Stadi-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Profile fitted scans $2\theta/\omega$=1/1
Absorption correction: numerical (North *et al.*, 1968)
T_{min} = 0.952, T_{max} = 0.968
1318 measured reflections
1188 independent reflections
1053 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 22.5°, θ_{min} = 2.7°
h = −14→14
k = 0→9
l = 0→9
3 standard reflections every 200 min
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
S = 1.10
1188 reflections
123 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.4775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}
Cl1	0.57659 (6)	0.28510 (10)	0.14255 (11)	0.0828 (3)
C2	0.49079 (17)	0.1523 (3)	0.1922 (3)	0.0513 (6)
H2A	0.5164	0.0516	0.1845	0.062*
H2B	0.4798	0.1684	0.3005	0.062*
C3	0.39513 (17)	0.1690 (3)	0.0802 (3)	0.0429 (6)
O4	0.39022 (12)	0.1400 (2)	−0.06122 (19)	0.0558 (5)
N5	0.31738 (15)	0.2133 (2)	0.1451 (3)	0.0453 (5)
H5N	0.327 (2)	0.249 (3)	0.240 (4)	0.054*
C6	0.22271 (18)	0.2355 (3)	0.0519 (3)	0.0427 (6)
C7	0.19078 (19)	0.3809 (3)	0.0168 (3)	0.0523 (6)
C8	0.0989 (2)	0.3999 (3)	−0.0760 (3)	0.0649 (8)

H8	0.0753	0.4963	−0.1002	0.078*
C9	0.0431 (2)	0.2789 (4)	−0.1320 (4)	0.0708 (9)
H9	−0.0176	0.2935	−0.1952	0.085*
C10	0.0758 (2)	0.1364 (4)	−0.0957 (3)	0.0646 (8)
H10	0.0369	0.0552	−0.1342	0.077*
C11	0.16630 (19)	0.1110 (3)	−0.0023 (3)	0.0520 (6)
C12	0.2526 (2)	0.5139 (3)	0.0770 (4)	0.0811 (9)
H12A	0.2218	0.6041	0.0322	0.097*
H12B	0.3166	0.5044	0.0468	0.097*
H12C	0.2588	0.5181	0.1905	0.097*
C13	0.2003 (2)	−0.0464 (3)	0.0398 (4)	0.0719 (8)
H13A	0.2543	−0.0711	−0.0143	0.086*
H13B	0.1471	−0.1152	0.0083	0.086*
H13C	0.2211	−0.0536	0.1522	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0568 (5)	0.1009 (7)	0.0869 (6)	−0.0204 (4)	−0.0005 (4)	0.0113 (4)
C2	0.0438 (13)	0.0629 (16)	0.0463 (13)	0.0064 (12)	0.0042 (11)	0.0048 (11)
C3	0.0452 (14)	0.0458 (14)	0.0374 (14)	0.0021 (11)	0.0058 (10)	0.0056 (10)
O4	0.0506 (10)	0.0790 (13)	0.0375 (10)	0.0091 (9)	0.0060 (7)	−0.0012 (8)
N5	0.0404 (12)	0.0594 (13)	0.0347 (10)	0.0028 (9)	0.0016 (9)	−0.0026 (9)
C6	0.0374 (14)	0.0539 (15)	0.0372 (11)	0.0012 (11)	0.0073 (11)	0.0023 (10)
C7	0.0493 (15)	0.0548 (15)	0.0522 (14)	0.0009 (12)	0.0062 (12)	0.0040 (12)
C8	0.0547 (17)	0.0666 (18)	0.0711 (17)	0.0146 (14)	0.0022 (14)	0.0140 (15)
C9	0.0447 (17)	0.094 (2)	0.0687 (18)	0.0043 (16)	−0.0070 (15)	0.0096 (16)
C10	0.0479 (16)	0.076 (2)	0.0657 (17)	−0.0097 (14)	−0.0029 (14)	−0.0065 (14)
C11	0.0483 (15)	0.0563 (15)	0.0505 (13)	−0.0007 (12)	0.0053 (12)	−0.0026 (12)
C12	0.085 (2)	0.0578 (18)	0.096 (2)	−0.0039 (16)	−0.0008 (18)	0.0036 (16)
C13	0.0662 (19)	0.0567 (17)	0.091 (2)	−0.0056 (14)	0.0051 (16)	−0.0014 (15)

Geometric parameters (Å, º)

Cl1—C2	1.770 (3)	C8—H8	0.9300
C2—C3	1.509 (3)	C9—C10	1.366 (4)
C2—H2A	0.9700	C9—H9	0.9300
C2—H2B	0.9700	C10—C11	1.389 (4)
C3—O4	1.227 (3)	C10—H10	0.9300
C3—N5	1.339 (3)	C11—C13	1.505 (4)
N5—C6	1.431 (3)	C12—H12A	0.9600
N5—H5N	0.86 (3)	C12—H12B	0.9600
C6—C7	1.386 (3)	C12—H12C	0.9600
C6—C11	1.391 (3)	C13—H13A	0.9600
C7—C8	1.394 (4)	C13—H13B	0.9600
C7—C12	1.501 (4)	C13—H13C	0.9600
C8—C9	1.367 (4)		

C3—C2—Cl1	109.33 (17)	C10—C9—C8	120.4 (3)
C3—C2—H2A	109.8	C10—C9—H9	119.8
Cl1—C2—H2A	109.8	C8—C9—H9	119.8
C3—C2—H2B	109.8	C9—C10—C11	121.1 (3)
Cl1—C2—H2B	109.8	C9—C10—H10	119.5
H2A—C2—H2B	108.3	C11—C10—H10	119.5
O4—C3—N5	123.0 (2)	C10—C11—C6	117.7 (2)
O4—C3—C2	120.8 (2)	C10—C11—C13	120.4 (2)
N5—C3—C2	116.2 (2)	C6—C11—C13	121.9 (2)
C3—N5—C6	121.9 (2)	C7—C12—H12A	109.5
C3—N5—H5N	119 (2)	C7—C12—H12B	109.5
C6—N5—H5N	117.6 (19)	H12A—C12—H12B	109.5
C7—C6—C11	122.1 (2)	C7—C12—H12C	109.5
C7—C6—N5	118.7 (2)	H12A—C12—H12C	109.5
C11—C6—N5	119.2 (2)	H12B—C12—H12C	109.5
C6—C7—C8	117.7 (2)	C11—C13—H13A	109.5
C6—C7—C12	121.3 (2)	C11—C13—H13B	109.5
C8—C7—C12	120.9 (3)	H13A—C13—H13B	109.5
C9—C8—C7	120.9 (3)	C11—C13—H13C	109.5
C9—C8—H8	119.5	H13A—C13—H13C	109.5
C7—C8—H8	119.5	H13B—C13—H13C	109.5

Cl1—C2—C3—O4	66.1 (3)	C6—C7—C8—C9	−0.9 (4)
Cl1—C2—C3—N5	−115.4 (2)	C12—C7—C8—C9	179.4 (3)
O4—C3—N5—C6	−2.4 (4)	C7—C8—C9—C10	1.0 (5)
C2—C3—N5—C6	179.1 (2)	C8—C9—C10—C11	−0.3 (5)
C3—N5—C6—C7	−103.9 (3)	C9—C10—C11—C6	−0.5 (4)
C3—N5—C6—C11	75.3 (3)	C9—C10—C11—C13	178.5 (3)
C11—C6—C7—C8	0.0 (4)	C7—C6—C11—C10	0.7 (4)
N5—C6—C7—C8	179.2 (2)	N5—C6—C11—C10	−178.5 (2)
C11—C6—C7—C12	179.7 (3)	C7—C6—C11—C13	−178.4 (3)
N5—C6—C7—C12	−1.1 (4)	N5—C6—C11—C13	2.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*N*···O4^{i}	0.86 (3)	2.04 (3)	2.866 (3)	161 (3)

Symmetry code: (i) $x, -y+1/2, z+1/2$.