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N-(2-Chlorophenyl)-2-methylbenzamide

B. Thimme Gowda,[a]* Sabine Foro,[b] B. P. Sowmya[a] and Hartmut Fuess[b]

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

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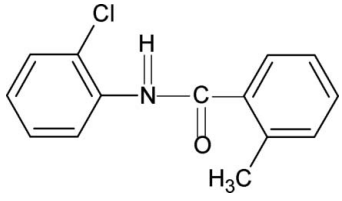
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.068; wR factor = 0.333; data-to-parameter ratio = 13.5.

In the structure of the title compound (N2CP2MBA), $C_{14}H_{12}ClNO$, the conformations of the N—H and C═O bonds are *trans* to each other. Furthermore, the conformation of the N—H bond is *syn* to the *ortho*-chloro group in the aniline ring and the C═O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring, similar to what is observed in 2-chloro-*N*-(2-chlorophenyl)benzamide and 2-methyl-*N*-phenylbenzamide. The amide group makes almost the same dihedral angles of 41.2 (14) and 42.2 (13)° with the aniline and benzoyl rings, respectively, while the dihedral angle between the benzoyl and aniline rings is only 7.4 (3)°. The molecules in N2CP2MBA are packed into chains through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003, 2008); Gowda, Foro *et al.* (2007); Gowda, Sowmya *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{12}ClNO$
M_r = 245.70
Monoclinic, $P2_1/n$
a = 4.8881 (4) Å
b = 24.318 (2) Å
c = 10.0562 (8) Å
β = 90.373 (6)°
V = 1195.34 (17) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.67 mm^{-1}
T = 299 (2) K
0.55 × 0.13 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.695, T_{max} = 0.878
2264 measured reflections
2126 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
3 standard reflections
frequency: 120 min
intensity decay: 1.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.333
S = 1.49
2126 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.88 (6)	2.03 (6)	2.886 (5)	163 (5)

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

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2196).

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supporting information

Acta Cryst. (2008). E**64**, o1421 [doi:10.1107/S1600536808020229]

N-(2-Chlorophenyl)-2-methylbenzamide

B. Thimme Gowda, Sabine Foro, B. P. Sowmya and Hartmut Fuess

S1. Comment

As part of a study of the substituent effects on the solid state geometries of benzanilides,in the present work, the structure of 2-methyl-*N*-(2-chlorophenyl)-benzamide (N2CP2MBA) has been determined Gowda *et al.* (2003, 2008). Gowda, Foro *et al.* (2007); Gowda, Sowmya *et al.* (2007). In the structure of N2CP2MBA (Fig. 1), the conformations of the N—H and C═O bonds are *trans* to each other. Further, the conformation of the N—H bond is *syn* to the *ortho*-chloro group in the aniline ring and that of the C═O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring. These observations are similar to those observed in 2-chloro-*N*-(2-Chlorophenyl)-benzamide (N2CP2CBA) (Gowda *et al.*, 2007*a*) and 2-methyl-*N*-(phenyl)-benzamide (NP2MBA) (Gowda *et al.*, 2008). The bond parameters in N2CP2MBA are similar to those in N2CP2CBA, NP2MBA, *N*-(2-Chlorophenyl)-benzamide and other benzanilides Gowda *et al.* (2003, 2008). Gowda, Foro *et al.* (2007); Gowda, Sowmya *et al.* (2007). The amide group, –NHCO– makes almost the same dihedral angles of 41.2 (14)° and 42.2 (13)° with the aniline and benzoyl rings, respectively, while that between the benzoyl and aniline rings is only 7.4 (3)°. The packing diagram of N2CP2MBA molecules showing the hydrogen bonds N—H···O (Table 1) involved in the formation of molecular chains is shown in Fig. 2.

S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. 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 NH atom was located in difference map and refined with a restrained N—H = 0.88 (6) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom). In spite of the refinement proceeding and converging smoothly, the R2 index did not decrese from a rather large value (0.33). This might be atributed to poor crystal quality in the available samples.

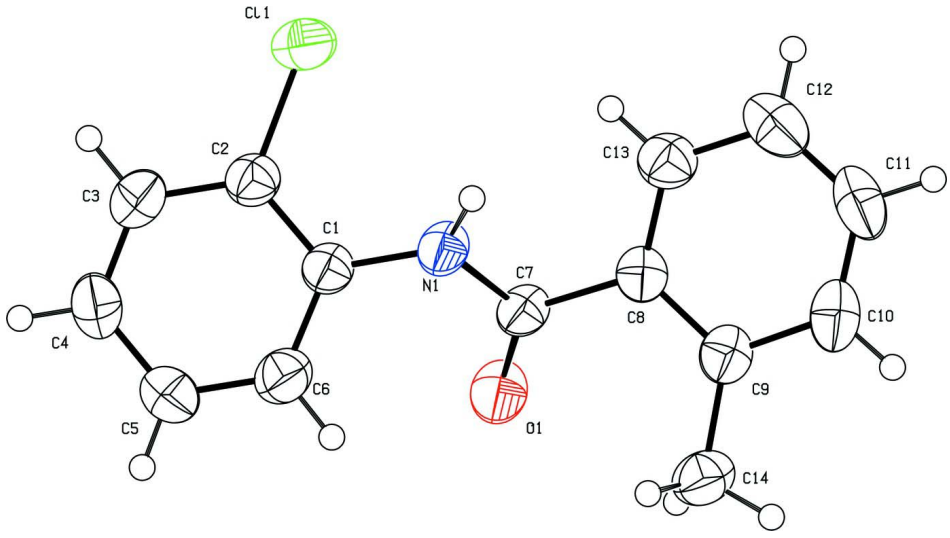

Figure 1

Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids drawn at the 50% probability level.

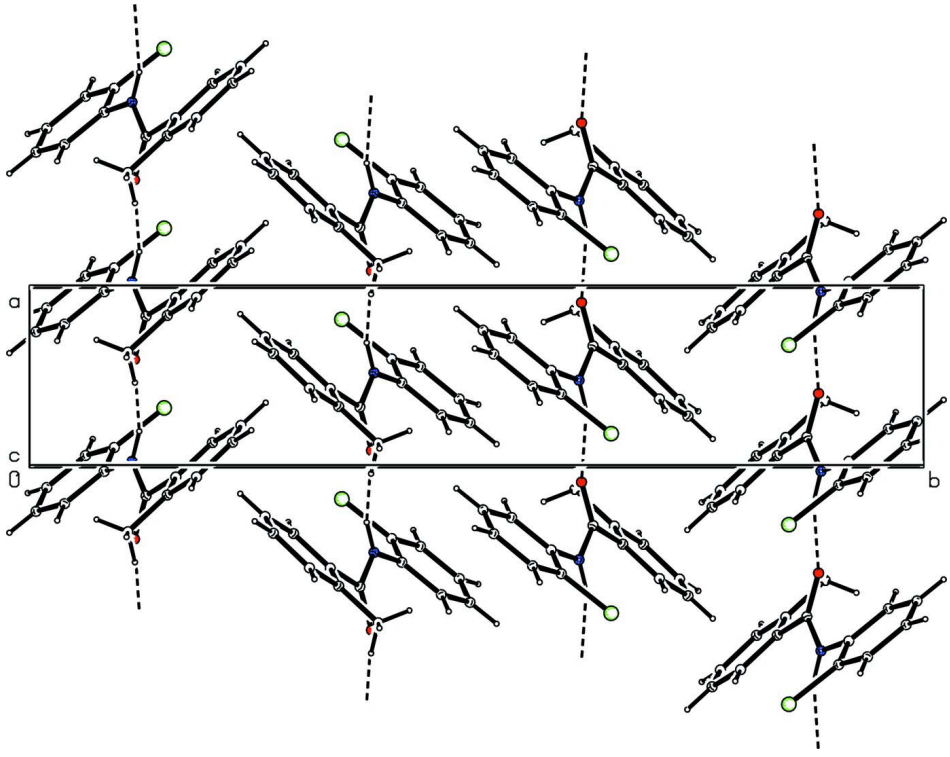

Figure 2

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

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Crystal data

$C_{14}H_{12}ClNO$
$M_r = 245.70$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.8881$ (4) Å
$b = 24.318$ (2) Å
$c = 10.0562$ (8) Å
$\beta = 90.373$ (6)°
$V = 1195.34$ (17) Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.365$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 7.3$–$21.6°$
$\mu = 2.67$ mm^{-1}
$T = 299$ K
Rod, colourless
0.55 × 0.13 × 0.05 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)
$T_{min} = 0.695$, $T_{max} = 0.878$
2264 measured reflections
2126 independent reflections
1695 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 66.9°$, $\theta_{min} = 3.6°$
$h = -5 \rightarrow 5$
$k = -29 \rightarrow 0$
$l = -12 \rightarrow 1$
3 standard reflections every 120 min
intensity decay: 1.5%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.333$
$S = 1.49$
2126 reflections
158 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
$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ 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}
C1	0.5268 (8)	0.58356 (18)	0.9109 (4)	0.0391 (10)
C2	0.3925 (9)	0.59484 (18)	0.7921 (5)	0.0435 (10)
C3	0.4354 (12)	0.5627 (2)	0.6800 (5)	0.0561 (13)

H3	0.3425	0.5707	0.6014	0.067*
C4	0.6138 (13)	0.5193 (2)	0.6847 (5)	0.0623 (15)
H4	0.6438	0.4981	0.6092	0.075*
C5	0.7482 (11)	0.5073 (2)	0.8016 (5)	0.0576 (13)
H5	0.8674	0.4776	0.8058	0.069*
C6	0.7067 (10)	0.5393 (2)	0.9124 (5)	0.0514 (12)
H6	0.8014	0.5311	0.9904	0.062*
C7	0.6651 (8)	0.63040 (19)	1.1158 (4)	0.0392 (10)
C8	0.5627 (8)	0.66363 (17)	1.2305 (4)	0.0377 (10)
C9	0.6654 (10)	0.65413 (18)	1.3586 (5)	0.0443 (11)
C10	0.5648 (11)	0.6868 (2)	1.4611 (5)	0.0554 (13)
H10	0.6293	0.6812	1.5473	0.067*
C11	0.3720 (12)	0.7272 (2)	1.4380 (6)	0.0632 (15)
H11	0.3062	0.7481	1.5083	0.076*
C12	0.2767 (11)	0.7365 (2)	1.3106 (6)	0.0608 (14)
H12	0.1495	0.7642	1.2945	0.073*
C13	0.3710 (10)	0.7046 (2)	1.2075 (5)	0.0493 (11)
H13	0.3054	0.7106	1.1216	0.059*
C14	0.8698 (11)	0.6100 (2)	1.3901 (5)	0.0549 (13)
H14A	1.0390	0.6179	1.3461	0.066*
H14B	0.8010	0.5751	1.3599	0.066*
H14C	0.9004	0.6086	1.4844	0.066*
N1	0.4730 (7)	0.61465 (17)	1.0252 (4)	0.0439 (9)
H1N	0.306 (13)	0.623 (2)	1.050 (5)	0.053*
O1	0.9068 (6)	0.61743 (16)	1.1044 (3)	0.0565 (10)
Cl1	0.1723 (3)	0.65063 (6)	0.78357 (13)	0.0601 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.027 (2)	0.052 (2)	0.038 (2)	0.0007 (16)	0.0020 (16)	−0.0012 (17)
C2	0.037 (2)	0.050 (2)	0.043 (2)	0.0006 (18)	−0.0003 (18)	0.0006 (19)
C3	0.057 (3)	0.067 (3)	0.044 (2)	0.005 (2)	−0.011 (2)	−0.004 (2)
C4	0.067 (3)	0.070 (3)	0.050 (3)	0.011 (3)	0.001 (2)	−0.019 (2)
C5	0.058 (3)	0.058 (3)	0.057 (3)	0.016 (2)	0.003 (2)	−0.005 (2)
C6	0.045 (3)	0.065 (3)	0.044 (2)	0.005 (2)	−0.0031 (19)	0.001 (2)
C7	0.025 (2)	0.058 (3)	0.035 (2)	−0.0011 (17)	0.0025 (16)	0.0022 (18)
C8	0.0257 (19)	0.046 (2)	0.041 (2)	−0.0081 (16)	0.0057 (16)	−0.0031 (18)
C9	0.040 (2)	0.053 (3)	0.041 (2)	−0.0059 (18)	0.0039 (19)	−0.0012 (18)
C10	0.058 (3)	0.065 (3)	0.044 (2)	−0.014 (2)	0.004 (2)	−0.014 (2)
C11	0.058 (3)	0.064 (3)	0.067 (3)	−0.001 (2)	0.014 (3)	−0.028 (3)
C12	0.048 (3)	0.048 (3)	0.086 (4)	0.001 (2)	0.005 (3)	−0.015 (2)
C13	0.039 (2)	0.057 (3)	0.052 (3)	0.0017 (19)	0.002 (2)	0.001 (2)
C14	0.044 (3)	0.072 (3)	0.048 (3)	0.006 (2)	−0.003 (2)	0.007 (2)
N1	0.0276 (18)	0.066 (2)	0.0378 (19)	0.0020 (16)	−0.0001 (15)	−0.0057 (17)
O1	0.0251 (16)	0.092 (3)	0.0523 (19)	0.0015 (16)	0.0009 (13)	−0.0153 (18)
Cl1	0.0564 (9)	0.0687 (10)	0.0551 (9)	0.0175 (5)	−0.0062 (6)	0.0061 (5)

Geometric parameters (Å, º)

C1—C2	1.387 (6)	C8—C13	1.386 (7)
C1—C6	1.390 (7)	C8—C9	1.399 (6)
C1—N1	1.402 (5)	C9—C10	1.394 (6)
C2—C3	1.388 (7)	C9—C14	1.499 (7)
C2—Cl1	1.734 (5)	C10—C11	1.380 (8)
C3—C4	1.369 (7)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.379 (8)
C4—C5	1.375 (8)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.377 (7)
C5—C6	1.374 (7)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14A	0.9600
C7—O1	1.229 (5)	C14—H14B	0.9600
C7—N1	1.359 (5)	C14—H14C	0.9600
C7—C8	1.497 (6)	N1—H1N	0.88 (6)
C2—C1—C6	117.3 (4)	C10—C9—C8	117.4 (5)
C2—C1—N1	120.6 (4)	C10—C9—C14	119.3 (4)
C6—C1—N1	122.1 (4)	C8—C9—C14	123.2 (4)
C1—C2—C3	121.0 (4)	C11—C10—C9	121.7 (5)
C1—C2—Cl1	119.2 (3)	C11—C10—H10	119.2
C3—C2—Cl1	119.8 (4)	C9—C10—H10	119.2
C4—C3—C2	120.4 (5)	C12—C11—C10	120.0 (5)
C4—C3—H3	119.8	C12—C11—H11	120.0
C2—C3—H3	119.8	C10—C11—H11	120.0
C3—C4—C5	119.6 (5)	C13—C12—C11	119.6 (5)
C3—C4—H4	120.2	C13—C12—H12	120.2
C5—C4—H4	120.2	C11—C12—H12	120.2
C6—C5—C4	120.1 (5)	C12—C13—C8	120.6 (5)
C6—C5—H5	120.0	C12—C13—H13	119.7
C4—C5—H5	120.0	C8—C13—H13	119.7
C5—C6—C1	121.7 (4)	C9—C14—H14A	109.5
C5—C6—H6	119.1	C9—C14—H14B	109.5
C1—C6—H6	119.1	H14A—C14—H14B	109.5
O1—C7—N1	121.7 (4)	C9—C14—H14C	109.5
O1—C7—C8	122.5 (4)	H14A—C14—H14C	109.5
N1—C7—C8	115.8 (3)	H14B—C14—H14C	109.5
C13—C8—C9	120.7 (4)	C7—N1—C1	124.7 (4)
C13—C8—C7	119.2 (4)	C7—N1—H1N	113 (3)
C9—C8—C7	120.0 (4)	C1—N1—H1N	122 (3)
C6—C1—C2—C3	0.5 (7)	C13—C8—C9—C10	0.8 (6)
N1—C1—C2—C3	−177.1 (4)	C7—C8—C9—C10	179.2 (4)
C6—C1—C2—Cl1	−178.4 (3)	C13—C8—C9—C14	179.1 (4)
N1—C1—C2—Cl1	3.9 (6)	C7—C8—C9—C14	−2.5 (6)
C1—C2—C3—C4	−0.5 (8)	C8—C9—C10—C11	−0.2 (7)

Cl1—C2—C3—C4	178.5 (4)	C14—C9—C10—C11	−178.6 (5)
C2—C3—C4—C5	0.7 (9)	C9—C10—C11—C12	−0.9 (8)
C3—C4—C5—C6	−1.0 (9)	C10—C11—C12—C13	1.3 (9)
C4—C5—C6—C1	1.1 (8)	C11—C12—C13—C8	−0.7 (8)
C2—C1—C6—C5	−0.8 (7)	C9—C8—C13—C12	−0.4 (7)
N1—C1—C6—C5	176.8 (5)	C7—C8—C13—C12	−178.8 (4)
O1—C7—C8—C13	139.0 (5)	O1—C7—N1—C1	−1.0 (7)
N1—C7—C8—C13	−41.8 (6)	C8—C7—N1—C1	179.8 (4)
O1—C7—C8—C9	−39.4 (6)	C2—C1—N1—C7	−141.4 (5)
N1—C7—C8—C9	139.8 (4)	C6—C1—N1—C7	41.1 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.88 (6)	2.03 (6)	2.886 (5)	163 (5)

Symmetry code: (i) *x*−1, *y*, *z*.