

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N-(3-Chlorophenyl)-2-methylbenzamide

B. Thimme Gowda,^{a*} Sabine Foro,^b B. P. Sowmya^a and Hartmut Fuess^b^aDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and ^bInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany

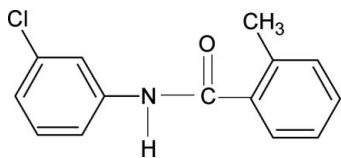
Correspondence e-mail: gowdabt@yahoo.com

Received 8 April 2008; accepted 14 April 2008

Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.043; wR factor = 0.121; data-to-parameter ratio = 13.7.

The conformation of the N—H bond in the structure of the title compound, $\text{C}_{14}\text{H}_{12}\text{ClNO}$, is *anti* to the *meta*-chloro substituent in the aniline ring, while the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring. The conformations of the N—H and C=O bonds are *anti* to each other, similar to those observed in 2-methyl-*N*-(3-methylphenyl)benzamide (N3MP2MBA). The —NHC(=O)— group makes a dihedral angle of $55.8(7)^\circ$ with the benzoyl ring, while the angle between the benzoyl and aniline rings is $37.5(1)^\circ$; the respective values for N3MP2MBA are $55.2(7)^\circ$ and $36.2(1)^\circ$. N—H \cdots O hydrogen bonds link the molecules into infinite chains running along the c axis.

Related literature

For related literature, see: Gowda *et al.* (2003, 2008a,b).

Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{ClNO}$
 $M_r = 245.70$
 Tetragonal, $P4_3$
 $a = 8.8237(8)$ Å

$c = 15.977(2)$ Å
 $V = 1243.9(2)$ Å³
 $Z = 4$
 Cu $K\alpha$ radiation

$\mu = 2.57$ mm⁻¹
 $T = 299(2)$ K

0.60 × 0.10 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.308$, $T_{\max} = 0.841$
 4144 measured reflections

2173 independent reflections
 1844 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 3 standard reflections
 frequency: 120 min
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.120$
 $S = 1.07$
 2173 reflections
 159 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³
 Absolute structure: Flack (1983), 1020 Friedel pairs
 Flack parameter: 0.00(2)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}^i$	0.83 (4)	2.12 (4)	2.900 (3)	157 (3)

Symmetry code: (i) $-y + 1, x, z - \frac{1}{4}$

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; 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: OM2228).

References

- Enraf–Nonius (1996). *CAD-4-PC*. Enraf–Nonius, Delft, The Netherlands.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Gowda, B. T., Foro, S., Sowmya, B. P. & Fuess, H. (2008a). *Acta Cryst.* **E64**, o383.
 Gowda, B. T., Foro, S., Sowmya, B. P. & Fuess, H. (2008b). *Acta Cryst.* **E64**, o541.
 Gowda, B. T., Jyothi, K., Paulus, H. & Fuess, H. (2003). *Z. Naturforsch. Teil A*, **58**, 225–230.
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Stoe & Cie (1987). *REDU4*. Stoe & Cie GmbH, Darmstadt, Germany.

supplementary materials

Acta Cryst. (2008). E64, o861 [doi:10.1107/S1600536808010143]

N-(3-Chlorophenyl)-2-methylbenzamide

B. T. Gowda, S. Foro, B. P. Sowmya and H. Fuess

Comment

In the present work, the structure of 2-methyl-*N*-(3-chlorophenyl)- benzamide (N3CP2MBA) has been determined as part of substituent effect studies on the solid state structures of benzanilides (Gowda *et al.*, 2003; Gowda *et al.* (2008a, 2008b). The conformation of the N—H bond in N3CP2MBA (Fig. 1) is *anti* to the *meta*-chloro substituent in the aniline ring, while the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring and the conformations of the N—H and C=O bonds are *anti* to each other, identical to that observed in 2-methyl-*N*-(3-methylphenyl)-benzamide (N3MP2MBA). The bond parameters in N3CP2MBA are similar to those in 2-methyl-*N*-(phenyl)-benzamide (Gowda *et al.*, 2008a), N3MP2MBA (Gowda *et al.*, 2008b) and other benzanilides (Gowda *et al.*, 2003). The amide group, —NHCO— makes a dihedral angle of 55.8 (7)° with the benzoyl ring, while that between benzoyl and aniline rings is 37.5 (1)°, compared to the respective values of 55.2 (7)° and 36.2 (1)° for N3MP2MBA. The packing diagram of N3CP2MBA showing the hydrogen bonds N1—H1N...O1 (Table 1) is given in Fig. 2.

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.

Refinement

The H on N1 was located in difference map and its position freely refined. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å and were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Figures

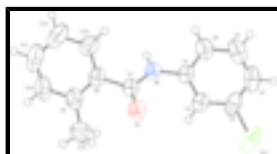


Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids drawn at the 50% probability level.

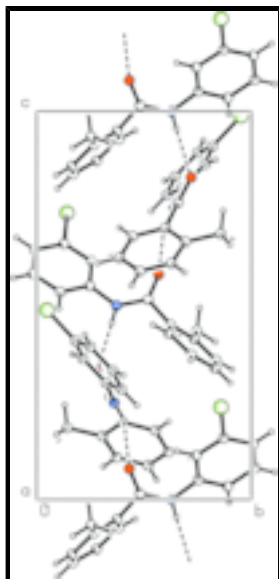


Fig. 2. Molecular packing of the title compound as viewed down *a* and with hydrogen bonding shown as dashed lines.

***N*-(3-Chlorophenyl)-2-methylbenzamide**

Crystal data

C₁₄H₁₂ClNO

M_r = 245.70

Tetragonal, *P*4₃

Hall symbol: *P* 4*cw*

a = 8.8237 (8) Å

b = 8.8237 (8) Å

c = 15.977 (2) Å

α = 90°

β = 90°

γ = 90°

V = 1243.9 (2) Å³

Z = 4

*F*₀₀₀ = 512

D_x = 1.312 Mg m⁻³

Cu *K*α radiation

λ = 1.54180 Å

Cell parameters from 25 reflections

θ = 5.7–21.9°

μ = 2.57 mm⁻¹

T = 299 (2) K

Rod, colourless

0.60 × 0.10 × 0.07 mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 299(2) K

ω/2θ scans

Absorption correction: Psi-scan
(North *et al.*, 1968)

T_{min} = 0.308, *T_{max}* = 0.841

4144 measured reflections

2173 independent reflections

R_{int} = 0.036

θ_{max} = 66.9°

θ_{min} = 5.0°

h = -10→10

k = -10→1

l = -19→16

3 standard reflections

every 120 min

intensity decay: none

1844 reflections with $I > 2\sigma(I)$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.019P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.120$	$(\Delta/\sigma)_{\max} = 0.025$
$S = 1.07$	$\Delta\rho_{\max} = 0.19 \text{ e } \text{Å}^{-3}$
2173 reflections	$\Delta\rho_{\min} = -0.29 \text{ e } \text{Å}^{-3}$
159 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.0079 (12)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1020 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.00 (2)

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6762 (3)	0.7532 (3)	0.05087 (15)	0.0463 (6)
C2	0.7849 (3)	0.7433 (3)	0.11372 (17)	0.0528 (6)
H2	0.8336	0.6521	0.1249	0.063*
C3	0.8186 (4)	0.8716 (4)	0.15884 (17)	0.0627 (8)
C4	0.7505 (5)	1.0087 (4)	0.1436 (2)	0.0763 (10)
H4	0.7762	1.0940	0.1747	0.092*
C5	0.6440 (5)	1.0169 (4)	0.0815 (2)	0.0831 (11)
H5	0.5963	1.1088	0.0705	0.100*
C6	0.6061 (4)	0.8896 (3)	0.0346 (2)	0.0673 (8)
H6	0.5337	0.8965	-0.0075	0.081*
C7	0.6591 (3)	0.4810 (3)	0.01510 (14)	0.0452 (5)
C8	0.5994 (3)	0.3752 (3)	-0.05047 (17)	0.0516 (6)
C9	0.6935 (4)	0.2659 (3)	-0.08605 (18)	0.0644 (8)

supplementary materials

C10	0.6279 (6)	0.1643 (4)	-0.1412 (2)	0.0887 (12)
H10	0.6885	0.0897	-0.1650	0.106*
C11	0.4808 (7)	0.1690 (4)	-0.1617 (3)	0.0992 (14)
H11	0.4415	0.0984	-0.1991	0.119*
C12	0.3864 (5)	0.2793 (5)	-0.1272 (3)	0.0955 (13)
H12	0.2841	0.2826	-0.1411	0.115*
C13	0.4472 (4)	0.3834 (4)	-0.0721 (2)	0.0695 (8)
H13	0.3863	0.4591	-0.0495	0.083*
C14	0.8575 (5)	0.2539 (5)	-0.0653 (3)	0.0923 (12)
H14A	0.8693	0.2414	-0.0059	0.111*
H14B	0.9088	0.3444	-0.0828	0.111*
H14C	0.9003	0.1680	-0.0936	0.111*
N1	0.6388 (3)	0.6279 (2)	-0.00053 (14)	0.0488 (5)
H1N	0.594 (4)	0.650 (3)	-0.045 (2)	0.059*
O1	0.7197 (2)	0.4315 (2)	0.07953 (11)	0.0598 (5)
Cl1	0.95205 (13)	0.85850 (13)	0.23813 (6)	0.0996 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0581 (14)	0.0483 (13)	0.0324 (12)	-0.0062 (11)	0.0045 (10)	0.0009 (10)
C2	0.0615 (15)	0.0546 (14)	0.0421 (13)	-0.0076 (11)	0.0013 (11)	0.0021 (11)
C3	0.0766 (18)	0.0721 (19)	0.0394 (15)	-0.0252 (15)	0.0044 (13)	-0.0071 (13)
C4	0.115 (3)	0.0605 (18)	0.0538 (19)	-0.0194 (18)	0.0127 (18)	-0.0145 (15)
C5	0.125 (3)	0.0505 (15)	0.074 (2)	0.0089 (18)	0.012 (2)	-0.0043 (16)
C6	0.092 (2)	0.0568 (16)	0.0532 (17)	0.0043 (14)	-0.0034 (16)	0.0023 (13)
C7	0.0528 (13)	0.0500 (13)	0.0327 (13)	-0.0022 (10)	0.0041 (10)	0.0020 (10)
C8	0.0721 (17)	0.0465 (13)	0.0361 (13)	-0.0069 (11)	-0.0036 (11)	0.0030 (10)
C9	0.094 (2)	0.0559 (15)	0.0434 (15)	0.0070 (15)	-0.0037 (14)	-0.0022 (12)
C10	0.149 (4)	0.0572 (18)	0.059 (2)	0.006 (2)	-0.020 (2)	-0.0159 (15)
C11	0.162 (4)	0.064 (2)	0.071 (2)	-0.034 (3)	-0.034 (3)	-0.0049 (18)
C12	0.103 (3)	0.095 (3)	0.089 (3)	-0.039 (2)	-0.039 (2)	0.009 (2)
C13	0.0712 (19)	0.0665 (17)	0.071 (2)	-0.0106 (15)	-0.0094 (15)	0.0044 (15)
C14	0.099 (3)	0.109 (3)	0.069 (2)	0.035 (2)	0.0100 (19)	-0.012 (2)
N1	0.0627 (13)	0.0512 (11)	0.0324 (10)	0.0005 (9)	-0.0063 (10)	0.0014 (9)
O1	0.0893 (13)	0.0559 (10)	0.0342 (10)	0.0054 (9)	-0.0073 (9)	0.0033 (8)
Cl1	0.1114 (7)	0.1195 (8)	0.0678 (6)	-0.0442 (6)	-0.0276 (5)	-0.0081 (5)

Geometric parameters (\AA , $^\circ$)

C1—C6	1.377 (4)	C8—C13	1.388 (4)
C1—C2	1.391 (4)	C8—C9	1.394 (4)
C1—N1	1.416 (3)	C9—C10	1.384 (5)
C2—C3	1.374 (4)	C9—C14	1.488 (5)
C2—H2	0.9300	C10—C11	1.339 (7)
C3—C4	1.373 (5)	C10—H10	0.9300
C3—Cl1	1.734 (3)	C11—C12	1.394 (7)
C4—C5	1.368 (6)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.382 (5)

C5—C6	1.392 (5)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14A	0.9600
C7—O1	1.240 (3)	C14—H14B	0.9600
C7—N1	1.332 (3)	C14—H14C	0.9600
C7—C8	1.499 (3)	N1—H1N	0.83 (4)
C6—C1—C2	120.0 (2)	C10—C9—C8	117.3 (3)
C6—C1—N1	117.9 (2)	C10—C9—C14	120.2 (3)
C2—C1—N1	122.0 (2)	C8—C9—C14	122.5 (3)
C3—C2—C1	118.4 (3)	C11—C10—C9	122.8 (4)
C3—C2—H2	120.8	C11—C10—H10	118.6
C1—C2—H2	120.8	C9—C10—H10	118.6
C4—C3—C2	122.6 (3)	C10—C11—C12	120.3 (3)
C4—C3—C11	119.1 (2)	C10—C11—H11	119.9
C2—C3—C11	118.4 (3)	C12—C11—H11	119.9
C5—C4—C3	118.4 (3)	C13—C12—C11	118.9 (4)
C5—C4—H4	120.8	C13—C12—H12	120.5
C3—C4—H4	120.8	C11—C12—H12	120.5
C4—C5—C6	120.8 (3)	C12—C13—C8	120.0 (4)
C4—C5—H5	119.6	C12—C13—H13	120.0
C6—C5—H5	119.6	C8—C13—H13	120.0
C1—C6—C5	119.7 (3)	C9—C14—H14A	109.5
C1—C6—H6	120.1	C9—C14—H14B	109.5
C5—C6—H6	120.1	H14A—C14—H14B	109.5
O1—C7—N1	123.8 (2)	C9—C14—H14C	109.5
O1—C7—C8	120.8 (2)	H14A—C14—H14C	109.5
N1—C7—C8	115.3 (2)	H14B—C14—H14C	109.5
C13—C8—C9	120.7 (3)	C7—N1—C1	128.3 (2)
C13—C8—C7	118.8 (3)	C7—N1—H1N	117 (2)
C9—C8—C7	120.5 (3)	C1—N1—H1N	115 (2)
C6—C1—C2—C3	0.5 (4)	C7—C8—C9—C10	174.9 (3)
N1—C1—C2—C3	177.7 (2)	C13—C8—C9—C14	179.4 (3)
C1—C2—C3—C4	-0.8 (4)	C7—C8—C9—C14	-3.6 (4)
C1—C2—C3—C11	179.1 (2)	C8—C9—C10—C11	0.9 (5)
C2—C3—C4—C5	0.7 (5)	C14—C9—C10—C11	179.5 (4)
C11—C3—C4—C5	-179.2 (3)	C9—C10—C11—C12	0.0 (6)
C3—C4—C5—C6	-0.4 (5)	C10—C11—C12—C13	0.3 (6)
C2—C1—C6—C5	-0.3 (5)	C11—C12—C13—C8	-1.4 (6)
N1—C1—C6—C5	-177.5 (3)	C9—C8—C13—C12	2.3 (5)
C4—C5—C6—C1	0.2 (6)	C7—C8—C13—C12	-174.7 (3)
O1—C7—C8—C13	121.7 (3)	O1—C7—N1—C1	-1.7 (4)
N1—C7—C8—C13	-56.8 (3)	C8—C7—N1—C1	176.9 (2)
O1—C7—C8—C9	-55.2 (3)	C6—C1—N1—C7	-160.9 (3)
N1—C7—C8—C9	126.2 (3)	C2—C1—N1—C7	21.9 (4)
C13—C8—C9—C10	-2.0 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
-------------------------	-------------	---------------	-----------------------	-------------------------

supplementary materials

N1—H1N···O1ⁱ 0.83 (4) 2.12 (4) 2.900 (3) 157 (3)
Symmetry codes: (i) $-y+1, x, z-1/4$.

Fig. 1

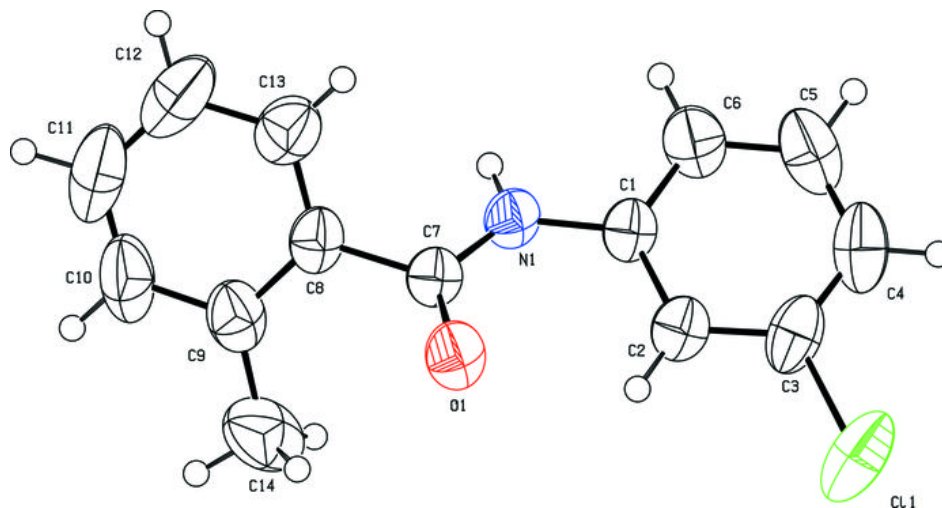


Fig. 2

