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N-(4-Chlorophenyl)-2-methylbenzamide

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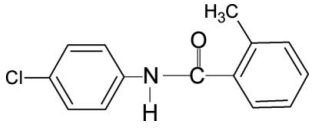
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.159; data-to-parameter ratio = 11.5.

In the structure of the title compound, $C_{14}H_{12}ClNO$, the N—H and C═O bonds are *trans* to each other. Furthermore, the C═O bond is *syn* to the *ortho*-methyl group in the benzoyl ring, similar to what is observed in 2-methyl-*N*-(4-methylphenyl)benzamide and 2-methyl-*N*-phenylbenzamide. The amide linkage (–NHCO–) makes dihedral angles of 36.9 (7) and 46.4 (5)° with the aniline and benzoyl rings, respectively, while the dihedral angle between the benzoyl and aniline rings is 83.1 (1)°. In the crystal structure, molecules form chains running along the *b* axis through N—H···O hydrogen bonds.

Related literature

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



Experimental

Crystal data

$C_{14}H_{12}ClNO$
M_r = 245.70
Monoclinic, $C2/c$
a = 22.345 (2) Å
b = 5.1092 (4) Å
c = 22.222 (1) Å
β = 109.593 (6)°
V = 2390.1 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 2.67 mm^{-1}
T = 299 (2) K
0.50 × 0.13 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2213 measured reflections
2085 independent reflections
1741 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.159
S = 1.08
2085 reflections
182 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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}	0.84 (3)	2.14 (3)	2.937 (3)	159 (2)

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2857).

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supplementary materials

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N-(4-Chlorophenyl)-2-methylbenzamide

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Comment

In the present work, as part of a study of the substituent effects on the solid state structures of benzanilides (Gowda *et al.*, 2003; 2008*a, b, c*), the structure of 2-methyl-*N*-(4-chlorophenyl)- benzamide has been determined. In the structure of the title compound (Fig. 1), the N—H and C=O bonds are *trans* to each other. Further, the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring. These observations are similar to those observed in 2-methyl-*N*-(phenyl)-benzamide (Gowda *et al.*, 2008*a*), 2-methyl-*N*-(4-methylphenyl)- benzamide (Gowda, Tokarčík *et al.*, 2008), 2-methyl-*N*- (2-chlorophenyl)-benzamide and 2-methyl-*N*-(3-chlorophenyl)- benzamide (Gowda *et al.*, 2008*b*). The amide linkage, –NHCO– makes dihedral angles of 36.9 (7)° and 46.4 (5)° with the aniline and benzoyl rings, respectively, while the dihedral angle between the benzoyl and aniline rings is 83.1 (1)°, in comparison with the central amide group –NHCO– being tilted to the benzoyl ring at an angle of 60.0 (1)° and the two rings (benzoyl & aniline) making a dihedral angle of 81.4 (1)° in N4MP2MBA. The other bond parameters in the title compound are similar to those in the previously mentioned structures. The packing diagram shows N—H···O (Table 1) hydrogen bonds connnecting the molecules into chains running along the b-axis (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 used in X-ray diffraction studies were obtained from a slow evaporation of its ethanolic solution at room temperature.

Refinement

The H atoms of the methyl group were positioned with idealized geometry using a riding model with C—H = 0.96 Å. The other H atoms were located in difference map, and their positional parameters were refined freely. The isotropic displacement parameters of all H atoms were set to 1.2 U_{eq}(C-aromatic, N) or 1.5 U_{eq}(C-methyl).

Figures

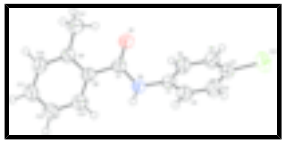

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

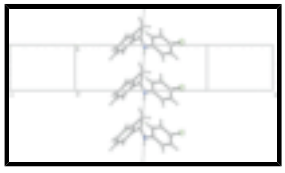

Fig. 2. Molecular packing of the title compound with hydrogen bonding shown as dashed lines..

N-(4-Chlorophenyl)-2-methylbenzamide

Crystal data

$C_{14}H_{12}ClNO$	F_{000} = 1024
M_r = 245.70	D_x = 1.366 Mg m^{-3}
Monoclinic, *C*2/*c*	Cu *K*α radiation λ = 1.54180 Å
Hall symbol: -C 2yc	Cell parameters from 25 reflections
a = 22.345 (2) Å	θ = 8.1–22.2º
b = 5.1092 (4) Å	μ = 2.67 mm^{-1}
c = 22.222 (1) Å	*T* = 299 (2) K
β = 109.593 (6)º	Rod, colourless
V = 2390.1 (3) Å^3	0.50 × 0.13 × 0.13 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.074
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 4.2º
T = 299(2) K	*h* = −25→26
ω/2θ scans	*k* = −6→0
Absorption correction: none	*l* = −26→1
2213 measured reflections	3 standard reflections
2085 independent reflections	every 120 min
1741 reflections with $I > 2\sigma(I)$	intensity decay: 1.0%

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
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$w = 1/[\sigma^2(F_o^2) + (0.1089P)^2 + 0.7738P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.159	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.08	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
2085 reflections	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
182 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0012 (3)
Secondary atom site location: difference Fourier map	

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	0.38579 (10)	−0.0174 (4)	0.97284 (10)	0.0427 (5)
C2	0.43053 (12)	−0.1978 (5)	0.96925 (11)	0.0531 (6)
H2	0.4467 (13)	−0.343 (6)	1.0021 (12)	0.064*
C3	0.45905 (12)	−0.1751 (6)	0.92298 (12)	0.0582 (6)
H3	0.4906 (14)	−0.296 (6)	0.9225 (13)	0.070*
C4	0.44190 (11)	0.0270 (5)	0.88024 (10)	0.0501 (6)
C5	0.39547 (13)	0.2001 (5)	0.88127 (11)	0.0556 (6)
H5	0.3833 (13)	0.344 (7)	0.8502 (13)	0.067*
C6	0.36711 (12)	0.1774 (5)	0.92743 (10)	0.0541 (6)
H6	0.3328 (14)	0.277 (6)	0.9283 (12)	0.065*
C7	0.34840 (11)	0.1669 (4)	1.05601 (10)	0.0464 (5)
C8	0.32646 (10)	0.0953 (4)	1.11029 (10)	0.0422 (5)
C9	0.35181 (9)	0.2246 (4)	1.16938 (9)	0.0437 (5)
C10	0.32915 (11)	0.1468 (5)	1.21792 (11)	0.0529 (6)
H10	0.3491 (12)	0.242 (6)	1.2606 (13)	0.063*
C11	0.28353 (12)	−0.0416 (5)	1.20908 (12)	0.0573 (6)
H11	0.2695 (14)	−0.099 (6)	1.2430 (14)	0.069*
C12	0.25847 (11)	−0.1652 (5)	1.15110 (12)	0.0567 (6)
H12	0.2257 (13)	−0.308 (6)	1.1438 (12)	0.068*
C13	0.28029 (11)	−0.0955 (5)	1.10188 (11)	0.0497 (5)
H13	0.2621 (12)	−0.182 (6)	1.0597 (12)	0.060*
C14	0.40270 (12)	0.4269 (5)	1.18350 (12)	0.0570 (6)
H14A	0.4283	0.4180	1.2278	0.068*
H14B	0.3837	0.5973	1.1741	0.068*
H14C	0.4288	0.3958	1.1576	0.068*
N1	0.36006 (10)	−0.0392 (4)	1.02268 (8)	0.0461 (5)
H1N	0.3609 (12)	−0.189 (6)	1.0382 (12)	0.055*
O1	0.35554 (12)	0.3935 (3)	1.04201 (9)	0.0740 (6)
Cl1	0.48134 (3)	0.07146 (16)	0.82524 (3)	0.0760 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0526 (11)	0.0351 (10)	0.0411 (10)	−0.0047 (9)	0.0164 (9)	−0.0033 (8)
C2	0.0640 (13)	0.0443 (13)	0.0541 (12)	0.0073 (10)	0.0240 (10)	0.0077 (10)
C3	0.0597 (13)	0.0582 (15)	0.0617 (14)	0.0086 (11)	0.0270 (11)	0.0013 (12)
C4	0.0588 (12)	0.0507 (13)	0.0445 (11)	−0.0110 (10)	0.0220 (10)	−0.0055 (9)
C5	0.0773 (15)	0.0458 (14)	0.0448 (11)	0.0035 (11)	0.0220 (10)	0.0053 (10)
C6	0.0688 (14)	0.0485 (14)	0.0479 (12)	0.0123 (11)	0.0233 (10)	0.0040 (10)
C7	0.0638 (12)	0.0334 (11)	0.0459 (11)	0.0005 (9)	0.0234 (9)	0.0011 (8)
C8	0.0485 (10)	0.0354 (11)	0.0447 (10)	0.0052 (8)	0.0185 (8)	0.0017 (8)
C9	0.0458 (10)	0.0394 (11)	0.0479 (11)	0.0053 (8)	0.0184 (8)	0.0003 (8)
C10	0.0592 (13)	0.0557 (14)	0.0485 (11)	0.0053 (11)	0.0245 (10)	−0.0031 (10)
C11	0.0628 (14)	0.0616 (15)	0.0590 (13)	0.0013 (11)	0.0358 (12)	0.0055 (11)
C12	0.0522 (12)	0.0537 (14)	0.0695 (15)	−0.0074 (11)	0.0274 (11)	0.0023 (12)
C13	0.0513 (11)	0.0461 (13)	0.0505 (11)	−0.0004 (10)	0.0155 (9)	0.0001 (10)
C14	0.0600 (13)	0.0505 (15)	0.0621 (13)	−0.0057 (10)	0.0226 (11)	−0.0080 (10)
N1	0.0669 (11)	0.0315 (9)	0.0455 (10)	0.0002 (8)	0.0262 (8)	0.0018 (7)
O1	0.1407 (18)	0.0319 (9)	0.0708 (11)	−0.0004 (10)	0.0636 (12)	0.0022 (7)
Cl1	0.0838 (5)	0.0892 (6)	0.0706 (5)	−0.0083 (4)	0.0465 (4)	0.0039 (4)

Geometric parameters (Å, °)

C1—C6	1.378 (3)	C8—C13	1.386 (3)
C1—C2	1.382 (3)	C8—C9	1.408 (3)
C1—N1	1.413 (3)	C9—C10	1.394 (3)
C2—C3	1.384 (3)	C9—C14	1.490 (3)
C2—H2	1.02 (3)	C10—C11	1.368 (4)
C3—C4	1.368 (4)	C10—H10	1.03 (3)
C3—H3	0.94 (3)	C11—C12	1.374 (4)
C4—C5	1.369 (4)	C11—H11	0.95 (3)
C4—Cl1	1.745 (2)	C12—C13	1.385 (3)
C5—C6	1.380 (3)	C12—H12	1.01 (3)
C5—H5	0.98 (3)	C13—H13	0.99 (3)
C6—H6	0.93 (3)	C14—H14A	0.9600
C7—O1	1.223 (3)	C14—H14B	0.9600
C7—N1	1.362 (3)	C14—H14C	0.9600
C7—C8	1.492 (3)	N1—H1N	0.84 (3)
C6—C1—C2	119.1 (2)	C10—C9—C8	116.8 (2)
C6—C1—N1	121.9 (2)	C10—C9—C14	119.0 (2)
C2—C1—N1	119.03 (19)	C8—C9—C14	124.18 (19)
C1—C2—C3	120.6 (2)	C11—C10—C9	122.4 (2)
C1—C2—H2	122.3 (15)	C11—C10—H10	122.6 (16)
C3—C2—H2	116.9 (15)	C9—C10—H10	115.0 (16)
C4—C3—C2	119.2 (2)	C10—C11—C12	120.5 (2)
C4—C3—H3	121.7 (17)	C10—C11—H11	122.0 (18)
C2—C3—H3	119.1 (17)	C12—C11—H11	117.4 (19)

C3—C4—C5	120.9 (2)	C11—C12—C13	118.8 (2)
C3—C4—Cl1	119.67 (19)	C11—C12—H12	122.0 (15)
C5—C4—Cl1	119.40 (19)	C13—C12—H12	119.2 (15)
C4—C5—C6	119.8 (2)	C12—C13—C8	121.2 (2)
C4—C5—H5	120.3 (17)	C12—C13—H13	119.4 (16)
C6—C5—H5	119.8 (17)	C8—C13—H13	119.4 (16)
C1—C6—C5	120.2 (2)	C9—C14—H14A	109.5
C1—C6—H6	115.6 (17)	C9—C14—H14B	109.5
C5—C6—H6	124.0 (17)	H14A—C14—H14B	109.5
O1—C7—N1	121.9 (2)	C9—C14—H14C	109.5
O1—C7—C8	122.95 (19)	H14A—C14—H14C	109.5
N1—C7—C8	115.14 (19)	H14B—C14—H14C	109.5
C13—C8—C9	120.3 (2)	C7—N1—C1	124.59 (19)
C13—C8—C7	119.68 (19)	C7—N1—H1N	117.7 (18)
C9—C8—C7	120.03 (19)	C1—N1—H1N	115.8 (18)
C6—C1—C2—C3	3.7 (4)	C7—C8—C9—C10	−179.84 (19)
N1—C1—C2—C3	−176.8 (2)	C13—C8—C9—C14	178.3 (2)
C1—C2—C3—C4	−0.7 (4)	C7—C8—C9—C14	−2.8 (3)
C2—C3—C4—C5	−2.4 (4)	C8—C9—C10—C11	−1.4 (3)
C2—C3—C4—Cl1	175.54 (19)	C14—C9—C10—C11	−178.6 (2)
C3—C4—C5—C6	2.5 (4)	C9—C10—C11—C12	0.7 (4)
Cl1—C4—C5—C6	−175.48 (19)	C10—C11—C12—C13	0.0 (4)
C2—C1—C6—C5	−3.7 (4)	C11—C12—C13—C8	−0.1 (4)
N1—C1—C6—C5	176.9 (2)	C9—C8—C13—C12	−0.6 (3)
C4—C5—C6—C1	0.6 (4)	C7—C8—C13—C12	−179.5 (2)
O1—C7—C8—C13	135.1 (3)	O1—C7—N1—C1	5.2 (4)
N1—C7—C8—C13	−44.8 (3)	C8—C7—N1—C1	−174.86 (18)
O1—C7—C8—C9	−43.7 (3)	C6—C1—N1—C7	−41.2 (3)
N1—C7—C8—C9	136.3 (2)	C2—C1—N1—C7	139.3 (2)
C13—C8—C9—C10	1.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.84 (3)	2.14 (3)	2.937 (3)	159 (2)

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

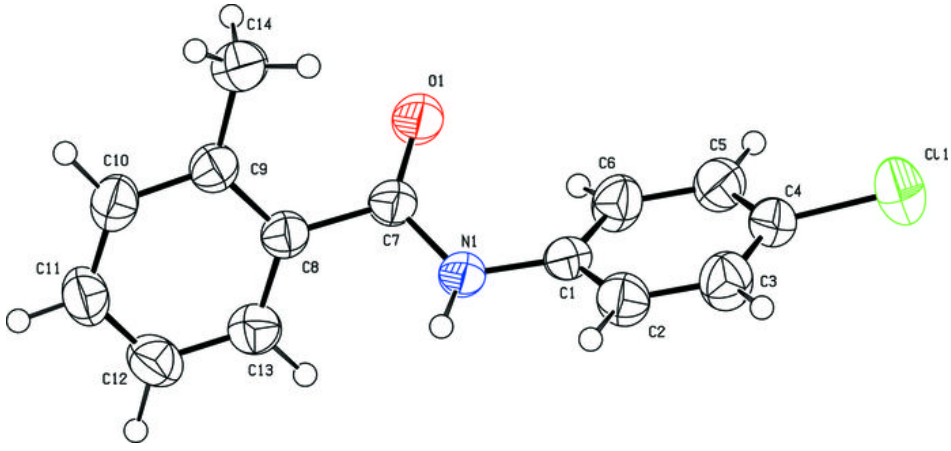

Fig. 2