Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2-Chlorophenyl)benzamide

B. Thimme Gowda,[a]* B. P. Sowmya,[a] Jozef Kožíšek,[b] Miroslav Tokarčík[c] and Hartmut Fuess[d]

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, [b]Department of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, [c]Department of Chemical Physics, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, and [d]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

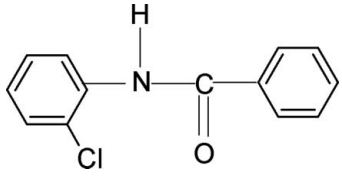
Received 4 May 2007; accepted 9 May 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.171; data-to-parameter ratio = 14.6.

In the structure of the title compound (N2CPBA), $C_{13}H_{10}ClNO$, the conformation of the N—H bond is *anti* to the *ortho*-Cl substituent in the aniline benzene ring. It closely resembles the structure of 2-chloro-*N*-phenylbenzamide (NP2CBA), although the two amides crystallize in different crystal systems. The molecules of N2CPBA are linked into a chain through an N—H···O hydrogen bond.

Related literature

For related literature, see: Gowda *et al.* (2003); Gowda, Foro & Fuess (2007); Gowda, Kozisek, Svoboda & Fuess (2007); Gowda *et al.* (2007*a*, 2007*b*).



Experimental

Crystal data

$C_{13}H_{10}ClNO$
M_r = 231.67
Orthorhombic, *Pbca*
a = 8.1122 (2) Å
b = 9.3093 (2) Å
c = 30.2818 (8) Å
V = 2286.85 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 295 (2) K
0.44 × 0.10 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.879, T_{max} = 0.994
23061 measured reflections
2224 independent reflections
1630 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.171
S = 1.11
2224 reflections
152 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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}	0.86	2.15	2.860 (2)	139

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship. JK and MT thank the Grant Agency of the Slovak Republic (grant No. 1/2449/05).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2106).

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  doi:10.1107/S1600536807022878

supplementary materials

Acta Cryst. (2007). E**63**, o2906 [**doi:10.1107/S1600536807022878**]

N-(2-Chlorophenyl)benzamide

B. T. Gowda, B. P. Sowmya, J. Kozísek, M. Tokarcík and H. Fuess

Comment

In the present work, the structure of *N*-(2-chlorophenyl)-benzamide (N2CPBA) has been determined to explore the substituent effects on the structure of N-aromatic amides (Gowda *et al.*, 2003; 2007*a*-*d*). In the structure of N2CPBA the N—H bond is anti to the *ortho*-Cl substituent in the aniline phenyl ring (Fig. 1). The structure of N2CPBA closely resembles the structure of *N*-(phenyl)-2-chlorobenzamide (NP2CBA) (Gowda *et al.*, 2003), although the two amides, N2CPBA and NP2CBA crystallize in different crystal systems: orthorhombic Pbca and tetragonal $P4_3$ space groups, respectively. The packing diagram of N2CPBA molecules showing the hydrogen bonds N1—H1N···O1^{i}, generating a chain along [010] [symmetry operation (i): $-x + 1/2, y + 1/2, z$] (Table 1, Fig. 2).

Experimental

The title compound was prepared according to the literature (Gowda *et al.*, 2003). The purity of the compound was checked by its melting point. It was characterized by IR and NMR spectra. Single crystals of the title compound were obtained from an ethanolic solution at room temperature and used for X-ray diffraction studies.

Refinement

H atoms were placed geometrically and refined using a riding model with C—H distances 0.93 Å for the ring H atoms, and N—H 0.86Å for the NH hydrogen atom.

Figures

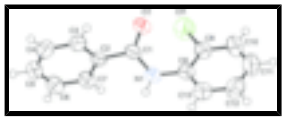

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

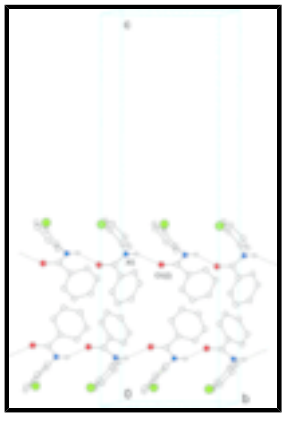

Fig. 2. Detail of crystal packing showing the hydrogen bonds N1—H1N···O1 generating a chain along [010] [symmetry operation: (i) $-x + 1/2, y + 1/2, z$].

N-(2-Chlorophenyl)benzamide

Crystal data

$C_{13}H_{10}ClNO$	$F_{000} = 960$
$M_r = 231.67$	$D_x = 1.346$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3908 reflections
$a = 8.1122$ (2) Å	$\theta = 3.2$–29.5°
$b = 9.3093$ (2) Å	$\mu = 0.31$ mm^{-1}
$c = 30.2818$ (8) Å	$T = 295$ (2) K
$V = 2286.85$ (10) Å^3	Prism, colourless
$Z = 8$	0.44 × 0.10 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur diffractometer	1630 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 295$(2) K	$\theta_{max} = 26.0^\circ$
φ scans, and ω scans with κ offsets	$\theta_{min} = 5.0^\circ$
Absorption correction: analytical (Clark & Reid, 1995)	$h = -9 \rightarrow 9$
$T_{min} = 0.879$, $T_{max} = 0.994$	$k = -11 \rightarrow 11$
23061 measured reflections	$l = -37 \rightarrow 37$
2224 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.171$	$w = 1/[\sigma^2(F_o^2) + (0.099P)^2 + 0.48P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} = 0.01$
2224 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
152 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.15606 (9)	0.39267 (9)	0.45504 (2)	0.0871 (3)
O1	0.16921 (19)	0.36964 (15)	0.35146 (6)	0.0637 (5)
N1	0.2540 (2)	0.58328 (16)	0.37875 (6)	0.0528 (5)
H1N	0.2364	0.6743	0.3799	0.063*
C1	0.1565 (2)	0.5005 (2)	0.35303 (6)	0.0476 (5)
C2	0.0327 (2)	0.57676 (19)	0.32524 (6)	0.0463 (5)
C3	−0.0134 (3)	0.5129 (2)	0.28601 (7)	0.0555 (5)
H3	0.035 (3)	0.423 (3)	0.2796 (8)	0.067*
C4	−0.1259 (3)	0.5798 (3)	0.25857 (8)	0.0644 (6)
H4	−0.1542	0.5378	0.2318	0.077*
C5	−0.1957 (3)	0.7079 (3)	0.27083 (9)	0.0704 (7)
H5	−0.2724	0.752	0.2525	0.085*
C6	−0.1530 (3)	0.7706 (3)	0.30982 (10)	0.0726 (7)
H6	−0.2016	0.8569	0.3181	0.087*
C7	−0.0373 (3)	0.7065 (2)	0.33722 (8)	0.0606 (6)
H7	−0.010 (3)	0.750 (3)	0.3651 (9)	0.073*
C8	0.3846 (3)	0.5237 (2)	0.40398 (6)	0.0511 (5)
C9	0.3559 (3)	0.4297 (2)	0.43837 (7)	0.0590 (6)
C10	0.4858 (4)	0.3669 (3)	0.46060 (9)	0.0776 (7)
H10	0.4648	0.3007	0.4829	0.093*
C11	0.6447 (4)	0.4011 (3)	0.45009 (10)	0.0819 (8)
H11	0.7317	0.3581	0.4651	0.098*
C12	0.6751 (3)	0.4993 (3)	0.41732 (10)	0.0781 (8)
H12	0.783	0.5251	0.4106	0.094*
C13	0.5455 (3)	0.5601 (3)	0.39423 (8)	0.0660 (6)
H13	0.567	0.6261	0.3719	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0785 (5)	0.1082 (7)	0.0747 (5)	−0.0152 (3)	0.0059 (3)	0.0285 (4)
O1	0.0778 (11)	0.0361 (8)	0.0771 (11)	0.0031 (6)	−0.0165 (8)	0.0041 (6)
N1	0.0603 (10)	0.0347 (8)	0.0634 (10)	0.0006 (7)	−0.0096 (8)	0.0067 (7)
C1	0.0520 (10)	0.0375 (10)	0.0534 (11)	−0.0006 (7)	0.0015 (8)	0.0060 (8)
C2	0.0462 (10)	0.0385 (9)	0.0541 (10)	−0.0032 (7)	0.0021 (8)	0.0085 (8)
C3	0.0528 (11)	0.0469 (11)	0.0670 (13)	−0.0038 (9)	−0.0023 (9)	−0.0007 (9)
C4	0.0628 (13)	0.0671 (14)	0.0634 (13)	−0.0115 (10)	−0.0128 (10)	0.0036 (11)

C5	0.0667 (13)	0.0571 (14)	0.0875 (16)	−0.0012 (11)	−0.0243 (12)	0.0165 (12)
C6	0.0749 (15)	0.0500 (12)	0.0930 (17)	0.0143 (10)	−0.0166 (12)	0.0027 (12)
C7	0.0662 (13)	0.0479 (11)	0.0678 (13)	0.0069 (9)	−0.0089 (10)	0.0018 (10)
C8	0.0581 (11)	0.0396 (10)	0.0556 (11)	−0.0012 (8)	−0.0048 (8)	0.0017 (8)
C9	0.0661 (13)	0.0558 (13)	0.0552 (12)	−0.0026 (9)	−0.0056 (9)	0.0056 (10)
C10	0.0890 (19)	0.0765 (16)	0.0673 (15)	0.0076 (14)	−0.0182 (13)	0.0206 (12)
C11	0.0736 (18)	0.087 (2)	0.0855 (19)	0.0151 (13)	−0.0237 (14)	0.0040 (15)
C12	0.0573 (13)	0.0841 (18)	0.0928 (19)	−0.0010 (12)	−0.0082 (12)	−0.0025 (15)
C13	0.0643 (14)	0.0599 (13)	0.0739 (14)	−0.0082 (10)	−0.0031 (11)	0.0062 (11)

Geometric parameters (Å, °)

Cl1—C9	1.733 (2)	C6—C7	1.387 (3)
O1—C1	1.224 (2)	C6—H6	0.93
N1—C1	1.351 (3)	C7—H7	0.96 (3)
N1—C8	1.419 (3)	C8—C9	1.379 (3)
N1—H1N	0.86	C8—C13	1.381 (3)
C1—C2	1.490 (3)	C9—C10	1.380 (3)
C2—C3	1.380 (3)	C10—C11	1.365 (4)
C2—C7	1.383 (3)	C10—H10	0.93
C3—C4	1.382 (3)	C11—C12	1.372 (4)
C3—H3	0.95 (3)	C11—H11	0.93
C4—C5	1.372 (4)	C12—C13	1.383 (4)
C4—H4	0.93	C12—H12	0.93
C5—C6	1.362 (4)	C13—H13	0.93
C5—H5	0.93		
C1—N1—C8	121.61 (16)	C2—C7—C6	119.8 (2)
C1—N1—H1N	119.2	C2—C7—H7	120.3 (15)
C8—N1—H1N	119.2	C6—C7—H7	119.8 (15)
O1—C1—N1	122.76 (18)	C9—C8—C13	118.5 (2)
O1—C1—C2	120.59 (18)	C9—C8—N1	121.90 (19)
N1—C1—C2	116.64 (16)	C13—C8—N1	119.65 (18)
C3—C2—C7	119.37 (19)	C8—C9—C10	120.6 (2)
C3—C2—C1	117.64 (17)	C8—C9—Cl1	120.24 (17)
C7—C2—C1	122.99 (18)	C10—C9—Cl1	119.18 (19)
C2—C3—C4	120.2 (2)	C11—C10—C9	120.5 (2)
C2—C3—H3	116.5 (15)	C11—C10—H10	119.7
C4—C3—H3	123.3 (15)	C9—C10—H10	119.7
C5—C4—C3	120.1 (2)	C10—C11—C12	119.6 (2)
C5—C4—H4	120	C10—C11—H11	120.2
C3—C4—H4	120	C12—C11—H11	120.2
C6—C5—C4	120.1 (2)	C11—C12—C13	120.1 (2)
C6—C5—H5	119.9	C11—C12—H12	119.9
C4—C5—H5	119.9	C13—C12—H12	119.9
C5—C6—C7	120.4 (2)	C8—C13—C12	120.7 (2)
C5—C6—H6	119.8	C8—C13—H13	119.7
C7—C6—H6	119.8	C12—C13—H13	119.7
C8—N1—C1—O1	3.6 (3)	C1—N1—C8—C9	−65.3 (3)
C8—N1—C1—C2	−175.03 (17)	C1—N1—C8—C13	114.8 (2)

O1—C1—C2—C3	−27.7 (3)	C13—C8—C9—C10	−4.0 (3)
N1—C1—C2—C3	151.00 (19)	N1—C8—C9—C10	176.1 (2)
O1—C1—C2—C7	151.9 (2)	C13—C8—C9—Cl1	174.40 (18)
N1—C1—C2—C7	−29.4 (3)	N1—C8—C9—Cl1	−5.5 (3)
C7—C2—C3—C4	1.4 (3)	C8—C9—C10—C11	2.6 (4)
C1—C2—C3—C4	−179.02 (19)	Cl1—C9—C10—C11	−175.8 (2)
C2—C3—C4—C5	−1.9 (3)	C9—C10—C11—C12	0.4 (5)
C3—C4—C5—C6	0.8 (4)	C10—C11—C12—C13	−1.9 (4)
C4—C5—C6—C7	0.7 (4)	C9—C8—C13—C12	2.5 (4)
C3—C2—C7—C6	0.1 (3)	N1—C8—C13—C12	−177.6 (2)
C1—C2—C7—C6	−179.4 (2)	C11—C12—C13—C8	0.4 (4)
C5—C6—C7—C2	−1.2 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.86	2.15	2.860 (2)	139

Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*.

Fig. 1

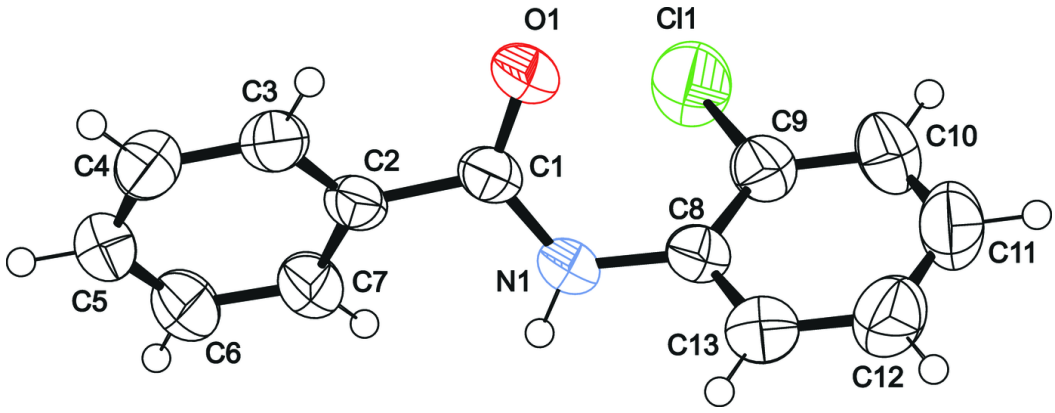

Fig. 2