

4-Chloro-*N*-phenylbenzamideVinola Z. Rodrigues,^a Lenka Kucková,^b B. Thimme Gowda^{a*} and Jozef Kožíšek^b

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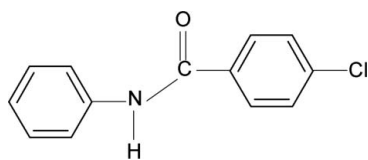
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 20.8.

In the title compound, $\text{C}_{13}\text{H}_{10}\text{ClNO}$, the dihedral angle between the two benzene rings is $59.6(1)^\circ$. The crystal structure features $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, which link the molecules into $C(4)$ chains running along the a axis.

Related literature

For the preparation of the title compound, see: Gowda *et al.* (2003). For our studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Bhat & Gowda (2000); Bowes *et al.* (2003); Gowda *et al.* (2008); Saeed *et al.* (2010), on *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007), on *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005) and on *N*-chloro-amides, Gowda & Weiss (1994).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{10}\text{ClNO}$ $\gamma = 90.023(4)^\circ$
 $M_r = 231.67$ $V = 544.64(5) \text{ \AA}^3$
 Triclinic, $P\bar{1}$ $Z = 2$
 $a = 5.3934(3) \text{ \AA}$ Mo $K\alpha$ radiation
 $b = 7.7679(5) \text{ \AA}$ $\mu = 0.33 \text{ mm}^{-1}$
 $c = 13.7831(8) \text{ \AA}$ $T = 298 \text{ K}$
 $\alpha = 105.887(5)^\circ$ $0.99 \times 0.51 \times 0.15 \text{ mm}$
 $\beta = 100.849(4)^\circ$

Data collection

Oxford Diffraction Xcalibur Ruby
 Gemini diffractometer
 Absorption correction: analytical
 [CrysAlis RED (Oxford
 Diffraction, 2009), based on
 expressions derived by Clark &
 Reid (1995)]
 $T_{\min} = 0.821$, $T_{\max} = 0.953$
 8972 measured reflections
 3010 independent reflections
 2330 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$ 145 parameters
 $wR(F^2) = 0.115$ H-atom parameters constrained
 $S = 1.07$ $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
 3010 reflections $\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.86	2.39	3.1987 (16)	157

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

Data collection: CrysAlis CCD (Oxford Diffraction, 2009); cell refinement: CrysAlis CCD; data reduction: CrysAlis RED (Oxford Diffraction, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2002); software used to prepare material for publication: enCIFer (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5692).

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supplementary materials

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4-Chloro-*N*-phenylbenzamide

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Comment

The amide moiety is the constituent of many biologically significant compounds. As part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Bhat & Gowda, 2000; Bowes *et al.*, 2003; Gowda *et al.*, 2008; Saeed *et al.*, 2010, *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005) and *N*-chloro-arylamides (Gowda & Weiss, 1994), in the present work, the crystal structure of *N*-(phenyl)-4-chlorobenzamide (I) has been determined (Fig.1).

In (I), the N—H and C=O bonds in the C—NH—C(O)—C segment are *anti* to each other, similar to that observed in *N*-(4-chlorophenyl)-benzamide (II)(Gowda *et al.*, 2008).

The dihedral angle between the two benzene rings is 59.6 (1)°, compared to the value of 60.8 (1)° in (II).

The packing of molecules linked by N—H···O hydrogen bonds into infinite chains is shown in Fig. 2.

Experimental

The title compound was prepared according to the method described by 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. Rod-like colourless single crystals of the title compound were obtained by slow evaporation from an ethanol solution of the compound (0.5 g in about 30 ml of ethanol) at room temperature.

Refinement

All H atoms were visible in difference maps and then treated as riding atoms with C—H distances of 0.93 Å (C-aromatic) and N—H = 0.86 Å. The $U_{\text{iso}}(\text{H})$ values were set at 1.2 $U_{\text{eq}}(\text{C-aromatic, N})$.

Figures

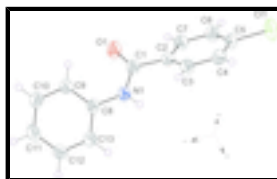


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

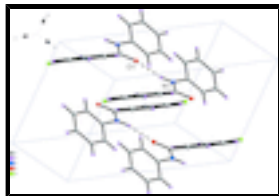


Fig. 2. Part of the crystal structure of the title compound. Molecular chains are generated by N—H...O hydrogen bonds which are shown by dashed lines.

4-Chloro-*N*-phenylbenzamide

Crystal data

$C_{13}H_{10}ClNO$	$Z = 2$
$M_r = 231.67$	$F(000) = 240$
Triclinic, $P\bar{1}$	$D_x = 1.413 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 5.3934 (3) \text{ \AA}$	Cell parameters from 3954 reflections
$b = 7.7679 (5) \text{ \AA}$	$\theta = 3.5\text{--}29.4^\circ$
$c = 13.7831 (8) \text{ \AA}$	$\mu = 0.33 \text{ mm}^{-1}$
$\alpha = 105.887 (5)^\circ$	$T = 298 \text{ K}$
$\beta = 100.849 (4)^\circ$	Plate, colourless
$\gamma = 90.023 (4)^\circ$	$0.99 \times 0.51 \times 0.15 \text{ mm}$
$V = 544.64 (5) \text{ \AA}^3$	

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer	3010 independent reflections
Radiation source: fine-focus sealed tube graphite	2330 reflections with $I > 2\sigma(I)$
Detector resolution: $10.4340 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.013$
ω scans	$\theta_{\text{max}} = 29.4^\circ$, $\theta_{\text{min}} = 3.5^\circ$
Absorption correction: analytical [CrysAlis RED (Oxford Diffraction, 2009), based on expressions derived by Clark & Reid (1995)]	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.821$, $T_{\text{max}} = 0.953$	$k = -10 \rightarrow 10$
8972 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.115$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.2195P]$
3010 reflections	where $P = (F_o^2 + 2F_c^2)/3$
	$(\Delta/\sigma)_{\text{max}} < 0.001$

145 parameters

$$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$$

0 restraints

$$\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. CrysAlis RED (Oxford Diffraction, 2009) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived (Clark & Reid, 1995).

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0813 (3)	0.2427 (2)	0.47100 (11)	0.0338 (3)
C2	0.0923 (3)	0.24248 (19)	0.36321 (11)	0.0309 (3)
C3	0.2913 (3)	0.3259 (2)	0.33873 (12)	0.0354 (3)
H3A	0.4279	0.3806	0.3902	0.042*
C4	0.2871 (3)	0.3280 (2)	0.23842 (12)	0.0381 (3)
H4A	0.4191	0.3849	0.2223	0.046*
C5	0.0845 (3)	0.2446 (2)	0.16262 (11)	0.0368 (3)
C6	-0.1146 (3)	0.1601 (2)	0.18473 (12)	0.0394 (3)
H6A	-0.2494	0.1037	0.1328	0.047*
C7	-0.1100 (3)	0.1608 (2)	0.28539 (12)	0.0358 (3)
H7A	-0.2442	0.1058	0.3013	0.043*
C8	0.3529 (3)	0.25180 (19)	0.63918 (11)	0.0302 (3)
C9	0.1937 (3)	0.3348 (2)	0.70443 (11)	0.0352 (3)
H9A	0.0466	0.3833	0.6787	0.042*
C10	0.2563 (3)	0.3443 (2)	0.80795 (12)	0.0397 (3)
H10A	0.1506	0.4001	0.8518	0.048*
C11	0.4737 (3)	0.2720 (2)	0.84716 (12)	0.0421 (4)
H11A	0.5144	0.2794	0.9169	0.050*
C12	0.6304 (3)	0.1886 (2)	0.78171 (13)	0.0410 (4)
H12A	0.7766	0.1392	0.8076	0.049*
C13	0.5711 (3)	0.1780 (2)	0.67819 (12)	0.0352 (3)
H13A	0.6771	0.1216	0.6346	0.042*
N1	0.3086 (2)	0.24555 (17)	0.53357 (9)	0.0340 (3)
H1A	0.4398	0.2433	0.5063	0.041*
O1	-0.1215 (2)	0.2392 (2)	0.49853 (9)	0.0507 (3)
Cl1	0.07987 (11)	0.24911 (8)	0.03678 (3)	0.06247 (18)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0306 (7)	0.0405 (8)	0.0314 (7)	0.0001 (6)	0.0075 (5)	0.0109 (6)
C2	0.0292 (6)	0.0351 (7)	0.0299 (7)	0.0041 (5)	0.0073 (5)	0.0105 (5)
C3	0.0301 (7)	0.0422 (8)	0.0342 (7)	-0.0018 (6)	0.0043 (6)	0.0126 (6)
C4	0.0367 (7)	0.0430 (8)	0.0397 (8)	0.0003 (6)	0.0129 (6)	0.0161 (7)
C5	0.0436 (8)	0.0413 (8)	0.0284 (7)	0.0086 (6)	0.0109 (6)	0.0121 (6)
C6	0.0364 (8)	0.0465 (8)	0.0317 (7)	-0.0011 (6)	0.0025 (6)	0.0080 (6)
C7	0.0294 (7)	0.0439 (8)	0.0347 (7)	-0.0020 (6)	0.0066 (6)	0.0116 (6)
C8	0.0285 (6)	0.0340 (7)	0.0292 (7)	-0.0019 (5)	0.0058 (5)	0.0106 (5)
C9	0.0306 (7)	0.0427 (8)	0.0339 (7)	0.0052 (6)	0.0082 (6)	0.0121 (6)
C10	0.0376 (8)	0.0496 (9)	0.0334 (8)	0.0020 (6)	0.0131 (6)	0.0101 (7)
C11	0.0410 (8)	0.0565 (10)	0.0313 (7)	-0.0044 (7)	0.0053 (6)	0.0177 (7)
C12	0.0319 (7)	0.0517 (9)	0.0427 (9)	0.0034 (6)	0.0031 (6)	0.0217 (7)
C13	0.0301 (7)	0.0414 (8)	0.0368 (8)	0.0041 (6)	0.0095 (6)	0.0132 (6)
N1	0.0285 (6)	0.0470 (7)	0.0293 (6)	0.0034 (5)	0.0081 (5)	0.0135 (5)
O1	0.0287 (5)	0.0897 (10)	0.0361 (6)	-0.0018 (6)	0.0085 (4)	0.0204 (6)
Cl1	0.0798 (4)	0.0789 (4)	0.0331 (2)	0.0003 (3)	0.0155 (2)	0.0199 (2)

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

C1—O1	1.2257 (17)	C8—C13	1.390 (2)
C1—N1	1.3558 (19)	C8—C9	1.391 (2)
C1—C2	1.4976 (19)	C8—N1	1.4173 (17)
C2—C7	1.389 (2)	C9—C10	1.384 (2)
C2—C3	1.3933 (19)	C9—H9A	0.9300
C3—C4	1.383 (2)	C10—C11	1.382 (2)
C3—H3A	0.9300	C10—H10A	0.9300
C4—C5	1.380 (2)	C11—C12	1.384 (2)
C4—H4A	0.9300	C11—H11A	0.9300
C5—C6	1.382 (2)	C12—C13	1.382 (2)
C5—Cl1	1.7398 (15)	C12—H12A	0.9300
C6—C7	1.382 (2)	C13—H13A	0.9300
C6—H6A	0.9300	N1—H1A	0.8600
C7—H7A	0.9300		
O1—C1—N1	123.61 (14)	C13—C8—C9	119.85 (13)
O1—C1—C2	121.13 (13)	C13—C8—N1	117.54 (12)
N1—C1—C2	115.26 (12)	C9—C8—N1	122.54 (13)
C7—C2—C3	119.09 (13)	C10—C9—C8	119.35 (14)
C7—C2—C1	118.05 (12)	C10—C9—H9A	120.3
C3—C2—C1	122.82 (13)	C8—C9—H9A	120.3
C4—C3—C2	120.48 (14)	C11—C10—C9	120.98 (14)
C4—C3—H3A	119.8	C11—C10—H10A	119.5
C2—C3—H3A	119.8	C9—C10—H10A	119.5
C5—C4—C3	119.13 (14)	C10—C11—C12	119.37 (15)
C5—C4—H4A	120.4	C10—C11—H11A	120.3

C3—C4—H4A	120.4	C12—C11—H11A	120.3
C4—C5—C6	121.55 (14)	C13—C12—C11	120.46 (14)
C4—C5—C11	118.82 (12)	C13—C12—H12A	119.8
C6—C5—C11	119.62 (12)	C11—C12—H12A	119.8
C7—C6—C5	118.82 (14)	C12—C13—C8	119.98 (14)
C7—C6—H6A	120.6	C12—C13—H13A	120.0
C5—C6—H6A	120.6	C8—C13—H13A	120.0
C6—C7—C2	120.92 (13)	C1—N1—C8	126.94 (12)
C6—C7—H7A	119.5	C1—N1—H1A	116.5
C2—C7—H7A	119.5	C8—N1—H1A	116.5
O1—C1—C2—C7	-28.3 (2)	C1—C2—C7—C6	178.28 (14)
N1—C1—C2—C7	151.19 (14)	C13—C8—C9—C10	0.7 (2)
O1—C1—C2—C3	149.28 (16)	N1—C8—C9—C10	-176.47 (14)
N1—C1—C2—C3	-31.2 (2)	C8—C9—C10—C11	-0.3 (2)
C7—C2—C3—C4	0.3 (2)	C9—C10—C11—C12	-0.2 (2)
C1—C2—C3—C4	-177.34 (14)	C10—C11—C12—C13	0.3 (2)
C2—C3—C4—C5	-0.7 (2)	C11—C12—C13—C8	0.1 (2)
C3—C4—C5—C6	0.4 (2)	C9—C8—C13—C12	-0.6 (2)
C3—C4—C5—C11	179.60 (12)	N1—C8—C13—C12	176.70 (13)
C4—C5—C6—C7	0.4 (2)	O1—C1—N1—C8	-2.5 (3)
C11—C5—C6—C7	-178.78 (12)	C2—C1—N1—C8	177.96 (13)
C5—C6—C7—C2	-0.9 (2)	C13—C8—N1—C1	152.65 (15)
C3—C2—C7—C6	0.6 (2)	C9—C8—N1—C1	-30.2 (2)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O1 ⁱ	0.86	2.39	3.1987 (16)	157.

Symmetry codes: (i) $x+1, y, z$.

Fig. 1

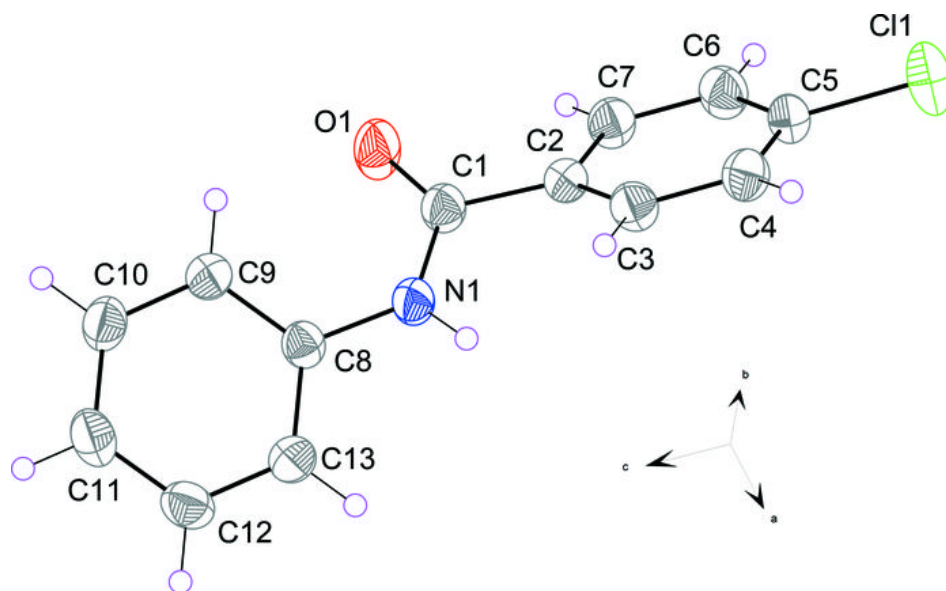


Fig. 2

