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N-(4-Chlorophenyl)-2-hydroxybenzamide

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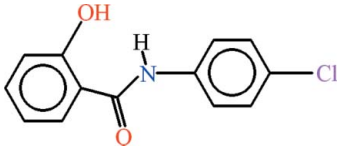
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 12.9.

In the title compound, $C_{13}H_{10}ClNO_2$, the dihedral angle between the aromatic rings is 20.02 (6)° and intramolecular N—H···O and C—H···O hydrogen bonds both generate S(6) rings. In the crystal, molecules are linked by O—H···O hydrogen bonds into C(6) chains propagating in [010].

Related literature

For biological background, see: Samanta *et al.* (2010). For related structures, see: Raza *et al.* (2009, 2010*a*,*b*). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_{10}ClNO_2$
M_r = 247.67
Orthorhombic, *Pbca*
a = 7.6832 (3) Å
b = 11.0225 (3) Å
c = 27.1427 (11) Å
V = 2298.66 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 296 K
0.28 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.942, T_{max} = 0.955
9244 measured reflections
2064 independent reflections
1561 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.03
2064 reflections
160 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.84 (2)	1.991 (18)	2.6588 (19)	136.4 (17)
O2—H2···O1^{i}	0.82 (2)	1.85 (2)	2.6582 (17)	173 (2)
C9—H9···O1	0.93	2.31	2.895 (2)	121

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. ARR also acknowledges the Higher Education Commission, Government of Pakistan, for generous support of a research project (20–819).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5690).

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supporting information

Acta Cryst. (2010). E**66**, o2922 [https://doi.org/10.1107/S1600536810042030]

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Abdul Rauf Raza, Bushra Nisar, M. Nawaz Tahir and Sumaira Shamshad

S1. Comment

Different synthetic derivatives of benzoxazepine have been reported as anti-tumor and anti-inflammatory agents (Samanta *et al.*, 2010). The title compound (I) was prepared as a precursor for the synthesis of chiral benzoxazepines and it will also be utilized for the complexation with various metals.

We have reported the crystal structures of (II) *i.e.*, 2-hydroxy-5-nitro-*N*-phenylbenzamide (Raza *et al.*, 2010*a*), (III) *i.e.*, 2-Hydroxy-*N*-(3-nitrophenyl)benzamide (Raza *et al.*, 2010*b*) and (IV) *i.e.*, 2-Hydroxy-3-nitro-*N*-phenylbenzamide (Raza *et al.*, 2009) which are related to the title compound.

In (I), the 2-hydroxyphenyl group A (C1–C6/O2) and 4-chloroanilinic group B (C8—C13/N1/CL1) are planar with r. m. s. deviation of 0.0072 and 0.0035 Å, respectively. The dihedral angle between A/B is 20.02 (6)°. There exist intramolecular H-bondings of N—H···O and C—H···O types (Table 1, Fig. 1) completing S(6) ring motifs (Bernstein *et al.*, 1995). The molecules are stabilized in the form of one dimensional polymeric chains extending along the crystallographic *b* axis due to intermolecular H-bondings of O—H···O type (Table 1, Fig. 2).

S2. Experimental

To a well stirred solution of 2-hydroxy benzoic acid (1.38 g, 0.01 mol, 1 eq) and $SOCl_2$ (0.87 ml, 1.42 g, 0.012 mol, 1.2 eq) in dry $CHCl_3$, the 4-chloroaniline (1.27 g, 0.01 mol, 1 eq) and Et_3N (2.08 ml, 1.5 g, 0.015 mol, 1.5 eq) was added slowly at room temperature followed by 3 h reflux. After commencement of reaction, the reaction mixture was cooled to room temperature, neutralized with aqueous $NaHCO_3$ (10%) and extracted with EtOAc (3×25 ml). The organic layer was combined, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure to afford light yellowish solid. The column chromatographic purification with 0 and 1% EtOAc in petrol (0.5 *L* each) over a silica gel packed column (of 25.5 cm length) afforded colorless prisms of (I) in 24th–106th fraction (10 ml each) upon leaving at room temperature.

S3. Refinement

The coordinates of H-atoms of amide and hydroxy group were refined. H atoms were positioned geometrically with (C–H = 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = xU_{eq}(C, N, O), where x = 1.2 for all H-atoms.

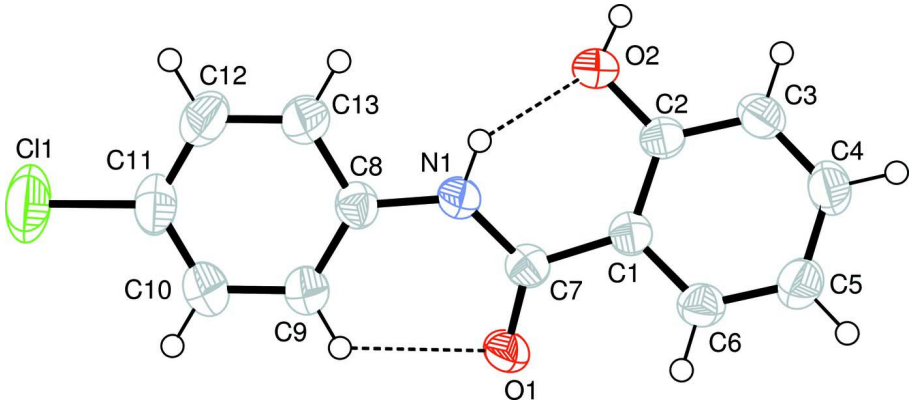

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radius. The dotted lines indicate the intramolecular H-bonds.

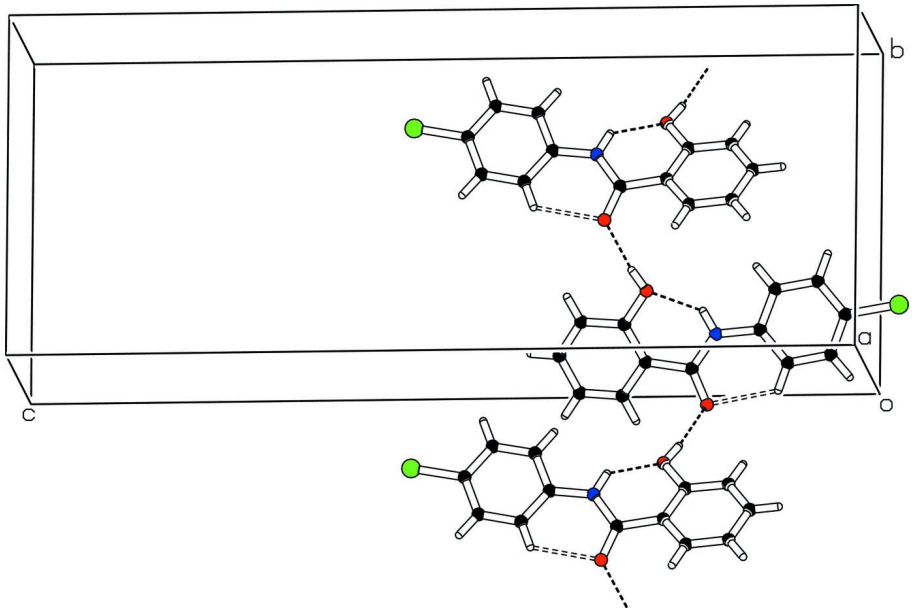

Figure 2

The partial packing for (I), which shows that molecules form one dimensional polymeric chains parallel to *b* axis.

N-(4-Chlorophenyl)-2-hydroxybenzamide

Crystal data

$C_{13}H_{10}ClNO_2$
$M_r = 247.67$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 7.6832\ (3)$ Å
$b = 11.0225\ (3)$ Å
$c = 27.1427\ (11)$ Å
$V = 2298.66\ (14)$ Å^3
$Z = 8$

$F(000) = 1024$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1561 reflections
$\theta = 3.0–25.3°$
$\mu = 0.32$ mm^{-1}
$T = 296$ K
Needle, colorless
0.28 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.5 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.942, T_{max} = 0.955

9244 measured reflections
2064 independent reflections
1561 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.3°, θ_{min} = 3.0°
h = −9→6
k = −13→11
l = −24→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.03
2064 reflections
160 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
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.540P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}
Cl1	0.37823 (11)	0.20751 (7)	−0.03285 (2)	0.0959 (3)
O1	0.33904 (17)	−0.07407 (10)	0.19332 (4)	0.0464 (4)
O2	0.52554 (18)	0.23574 (11)	0.26024 (5)	0.0482 (5)
N1	0.3890 (2)	0.12607 (13)	0.18202 (5)	0.0423 (5)
C1	0.3726 (2)	0.04847 (14)	0.26498 (6)	0.0355 (5)
C2	0.4477 (2)	0.14916 (14)	0.28844 (6)	0.0373 (6)
C3	0.4430 (3)	0.15880 (16)	0.33940 (6)	0.0461 (6)
C4	0.3619 (3)	0.07148 (18)	0.36719 (7)	0.0519 (7)
C5	0.2852 (3)	−0.02736 (17)	0.34495 (7)	0.0513 (7)
C6	0.2926 (2)	−0.03846 (15)	0.29454 (6)	0.0421 (6)
C7	0.3672 (2)	0.02787 (15)	0.21083 (6)	0.0369 (6)
C8	0.3852 (2)	0.13776 (15)	0.13042 (6)	0.0400 (6)
C9	0.3543 (3)	0.04338 (18)	0.09804 (7)	0.0552 (7)
C10	0.3524 (3)	0.0662 (2)	0.04786 (7)	0.0622 (8)
C11	0.3811 (3)	0.1803 (2)	0.03022 (7)	0.0569 (8)
C12	0.4125 (3)	0.27414 (19)	0.06207 (8)	0.0622 (8)

C13	0.4130 (3)	0.25274 (17)	0.11203 (7)	0.0529 (7)
H1	0.413 (2)	0.1904 (18)	0.1968 (7)	0.0508*
H2	0.565 (3)	0.291 (2)	0.2768 (8)	0.0723*
H3	0.49511	0.22482	0.35481	0.0553*
H4	0.35862	0.07910	0.40130	0.0623*
H5	0.22913	−0.08592	0.36383	0.0615*
H6	0.24253	−0.10608	0.27973	0.0505*
H9	0.33497	−0.03467	0.10984	0.0663*
H10	0.33127	0.00296	0.02596	0.0746*
H12	0.43326	0.35179	0.05002	0.0747*
H13	0.43238	0.31672	0.13369	0.0635*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1415 (7)	0.1043 (6)	0.0418 (3)	0.0140 (4)	−0.0015 (4)	0.0171 (3)
O1	0.0660 (9)	0.0328 (7)	0.0405 (7)	0.0004 (5)	−0.0077 (6)	−0.0046 (5)
O2	0.0679 (9)	0.0339 (7)	0.0428 (8)	−0.0089 (6)	−0.0031 (6)	−0.0018 (5)
N1	0.0591 (10)	0.0321 (8)	0.0358 (8)	0.0004 (7)	−0.0009 (7)	−0.0028 (6)
C1	0.0373 (9)	0.0326 (9)	0.0366 (9)	0.0072 (7)	0.0002 (7)	−0.0006 (7)
C2	0.0416 (10)	0.0296 (9)	0.0406 (10)	0.0064 (7)	−0.0003 (8)	0.0004 (7)
C3	0.0546 (12)	0.0406 (10)	0.0431 (10)	0.0015 (9)	−0.0044 (9)	−0.0076 (8)
C4	0.0661 (13)	0.0547 (12)	0.0349 (10)	0.0049 (10)	0.0035 (9)	−0.0031 (9)
C5	0.0592 (12)	0.0490 (12)	0.0456 (11)	−0.0030 (9)	0.0109 (9)	0.0038 (8)
C6	0.0441 (11)	0.0371 (10)	0.0450 (10)	−0.0014 (8)	0.0035 (8)	−0.0034 (8)
C7	0.0370 (10)	0.0341 (10)	0.0395 (10)	0.0058 (7)	−0.0015 (7)	−0.0010 (7)
C8	0.0425 (10)	0.0412 (10)	0.0364 (10)	0.0049 (8)	−0.0015 (8)	0.0001 (7)
C9	0.0797 (15)	0.0471 (12)	0.0389 (10)	−0.0058 (10)	0.0010 (10)	−0.0005 (8)
C10	0.0862 (16)	0.0611 (14)	0.0393 (11)	−0.0050 (11)	−0.0014 (10)	−0.0059 (9)
C11	0.0687 (14)	0.0661 (14)	0.0359 (11)	0.0103 (10)	0.0010 (10)	0.0072 (9)
C12	0.0852 (16)	0.0488 (12)	0.0527 (13)	0.0050 (10)	0.0011 (11)	0.0149 (10)
C13	0.0713 (14)	0.0409 (10)	0.0466 (12)	0.0039 (9)	−0.0017 (10)	0.0018 (8)

Geometric parameters (Å, º)

Cl1—C11	1.738 (2)	C8—C13	1.379 (3)
O1—C7	1.239 (2)	C8—C9	1.382 (3)
O2—C2	1.362 (2)	C9—C10	1.385 (3)
O2—H2	0.82 (2)	C10—C11	1.364 (3)
N1—C8	1.407 (2)	C11—C12	1.370 (3)
N1—C7	1.346 (2)	C12—C13	1.376 (3)
N1—H1	0.84 (2)	C3—H3	0.9300
C1—C6	1.393 (2)	C4—H4	0.9300
C1—C7	1.488 (2)	C5—H5	0.9300
C1—C2	1.404 (2)	C6—H6	0.9300
C2—C3	1.388 (2)	C9—H9	0.9300
C3—C4	1.372 (3)	C10—H10	0.9300
C4—C5	1.378 (3)	C12—H12	0.9300

C5—C6	1.375 (3)	C13—H13	0.9300
C2—O2—H2	112.1 (15)	Cl1—C11—C12	119.58 (17)
C7—N1—C8	130.51 (14)	Cl1—C11—C10	120.19 (16)
C8—N1—H1	113.9 (13)	C10—C11—C12	120.23 (18)
C7—N1—H1	115.5 (13)	C11—C12—C13	119.54 (19)
C2—C1—C6	117.65 (15)	C8—C13—C12	120.92 (18)
C2—C1—C7	125.47 (14)	C2—C3—H3	120.00
C6—C1—C7	116.86 (14)	C4—C3—H3	120.00
O2—C2—C3	121.20 (15)	C3—C4—H4	120.00
O2—C2—C1	118.67 (14)	C5—C4—H4	120.00
C1—C2—C3	120.13 (15)	C4—C5—H5	120.00
C2—C3—C4	120.39 (17)	C6—C5—H5	120.00
C3—C4—C5	120.52 (17)	C1—C6—H6	119.00
C4—C5—C6	119.25 (18)	C5—C6—H6	119.00
C1—C6—C5	122.03 (16)	C8—C9—H9	120.00
N1—C7—C1	116.60 (14)	C10—C9—H9	120.00
O1—C7—C1	121.48 (14)	C9—C10—H10	120.00
O1—C7—N1	121.89 (15)	C11—C10—H10	120.00
N1—C8—C9	124.58 (16)	C11—C12—H12	120.00
N1—C8—C13	116.19 (15)	C13—C12—H12	120.00
C9—C8—C13	119.22 (16)	C8—C13—H13	120.00
C8—C9—C10	119.36 (18)	C12—C13—H13	120.00
C9—C10—C11	120.73 (19)		
C8—N1—C7—O1	0.3 (3)	C1—C2—C3—C4	−1.4 (3)
C8—N1—C7—C1	−177.67 (16)	C2—C3—C4—C5	0.5 (3)
C7—N1—C8—C9	0.8 (3)	C3—C4—C5—C6	0.8 (3)
C7—N1—C8—C13	−179.92 (18)	C4—C5—C6—C1	−1.2 (3)
C6—C1—C2—O2	−179.53 (14)	N1—C8—C9—C10	179.49 (18)
C6—C1—C2—C3	0.9 (2)	C13—C8—C9—C10	0.2 (3)
C7—C1—C2—O2	−1.1 (2)	N1—C8—C13—C12	179.81 (19)
C7—C1—C2—C3	179.34 (16)	C9—C8—C13—C12	−0.8 (3)
C2—C1—C6—C5	0.4 (2)	C8—C9—C10—C11	0.2 (3)
C7—C1—C6—C5	−178.18 (16)	C9—C10—C11—Cl1	−179.98 (19)
C2—C1—C7—O1	161.80 (16)	C9—C10—C11—C12	0.1 (4)
C2—C1—C7—N1	−20.2 (2)	Cl1—C11—C12—C13	179.35 (18)
C6—C1—C7—O1	−19.8 (2)	C10—C11—C12—C13	−0.7 (4)
C6—C1—C7—N1	158.21 (15)	C11—C12—C13—C8	1.1 (3)
O2—C2—C3—C4	179.11 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.84 (2)	1.991 (18)	2.6588 (19)	136.4 (17)

O2—H2···O1^{i}	0.82 (2)	1.85 (2)	2.6582 (17)	173 (2)
C9—H9···O1	0.93	2.31	2.895 (2)	121

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