Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Hydroxy-*N*-(4-methylphenyl)-benzamide

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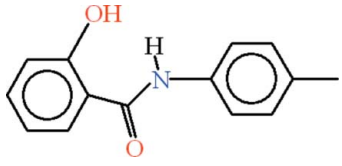
Received 25 July 2011; accepted 30 July 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.159; data-to-parameter ratio = 17.8.

In the crystal structure of the title compound, $C_{14}H_{13}NO_2$, the molecules are approximately planar, the r.m.s. deviation for all non-H atoms being 0.0435 Å; the dihedral angle between the two rings is 3.45 (12)°. The planarity is accounted for in terms of the presence of intramolecular N—H···O and C—H···O hydrogen bonding, each of which completes an S(6) ring motif. The molecules are stabilized in the form of supramolecular chains extending along the crystallographic c axis due to intermolecular O—H···O and C—H···O hydrogen bonding; each type leads to an $R_2^1(6)$ ring motif.

Related literature

For related benzamide structures, see: Raza *et al.* (2010*a*,*b*,*c*). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Monoclinic, $P2_1/c$
a = 19.4067 (17) Å
b = 4.9122 (5) Å
c = 12.7261 (11) Å
β = 104.793 (4)°
V = 1172.96 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.34 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.979, T_{max} = 0.988
10416 measured reflections
2771 independent reflections
1243 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.159
S = 0.96
2771 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.78	2.596 (2)	179
N1—H1A···O1	0.86	1.92	2.647 (2)	141
C3—H3···O2^{i}	0.93	2.51	3.179 (3)	129
C9—H9···O2	0.93	2.25	2.840 (3)	121

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

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 for Windows* (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, Ex-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: TK2771).

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supporting information

Acta Cryst. (2011). E**67**, o2253 [doi:10.1107/S1600536811030716]

2-Hydroxy-*N*-(4-methylphenyl)benzamide

Abdul Rauf Raza, Bushra Nisar and M. Nawaz Tahir

S1. Comment

We have reported the crystal structures of (II) *i.e*. 2-hydroxy-*N*-(3-nitrophenyl)benzamide (Raza *et al.*, 2010*a*), (III) *i.e*. *N*-(4-chlorophenyl)-2-hydroxybenzamide (Raza *et al.*, 2010*b*) and (IV) *i.e*. *N*-(3-chlorophenyl)-2 -hydroxybenzamide (Raza *et al.*, 2010*c*). In this connection, the title compound (I, Fig. 1) has been prepared as a precursor for the synthesis of symmetric as well as asymmetric benzoxazepines.

In (I), the 2-hydroxyphenyl group A (C1–C6/O1) and 4-methylanilinic group B (C8—C14/N1) are planar with r.m.s. deviations of 0.0048 and 0.0086 Å, respectively. The dihedral angle between A/B is 3.45 (12) °. There is intramolecular H-bonding of the type N—H···O and C—H···O types (Table 1, Fig. 1), each of which completes a *S*(6) ring motif (Bernstein *et al.*, 1995). There is also intermolecular H-bonding of the type C—H···O and O—H···O (Table 1). These lead to the formation of two $R_2^1(6)$ ring motifs and to supramolecular chains extending along the crystallographic *c*-axis (Fig. 2).

S2. Experimental

To a well stirred solution of 2-hydroxy benzoic acid (2.76 g, 0.02 mol, 1 equiv.) and $SOCl_2$ (1.74 mL, 2.84 g, 0.024 mol, 1.2 equiv.) in dry $CHCl_3$, 4-metylaniline (2.14 g, 0.02 mol, 1 equiv.) and Et_3N (4.16 mL, 3 g, 0.03 mol, 1.5 equiv.) were added slowly at room temperature followed by 3 h reflux. After completion of reaction, the reaction mixture was cooled to room temperature, neutralized with aqueous $NaHCO_3$ (10 %) and extracted with $CHCl_3$ (3×25 mL). The organic layers were combined, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure to afford a brown solid. The column chromatographic purification with 1%, 2% and 3% $CHCl_3$ in petrol (300 mL each) over a silica gel packed column (of 25.5 cm length) afforded white needles of (I) in the 96th-280th fractions (50 mL each).

S3. Refinement

Although H atoms appeared in difference Fourier maps they were positioned geometrically with (O–H = 0.82, N–H = 0.86 and C–H = 0.93-0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for hydroxy- & methyl-H atoms and x = 1.2 for other H atoms.

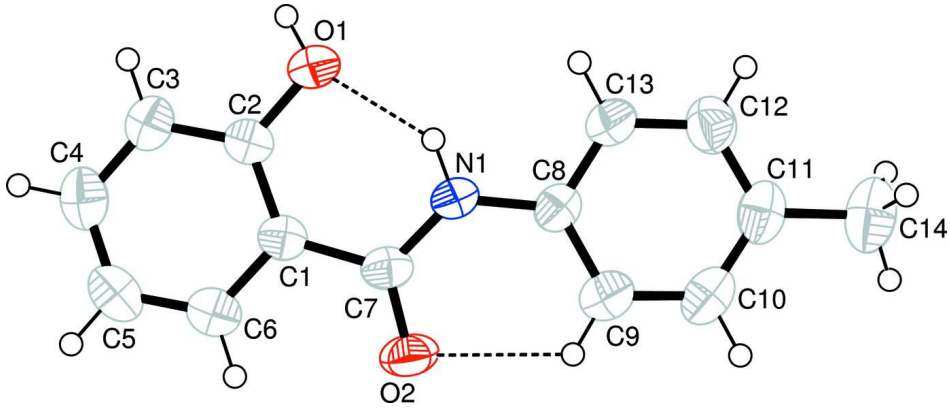

Figure 1

View of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii. The dotted line indicate the intramolecular H-bonding.

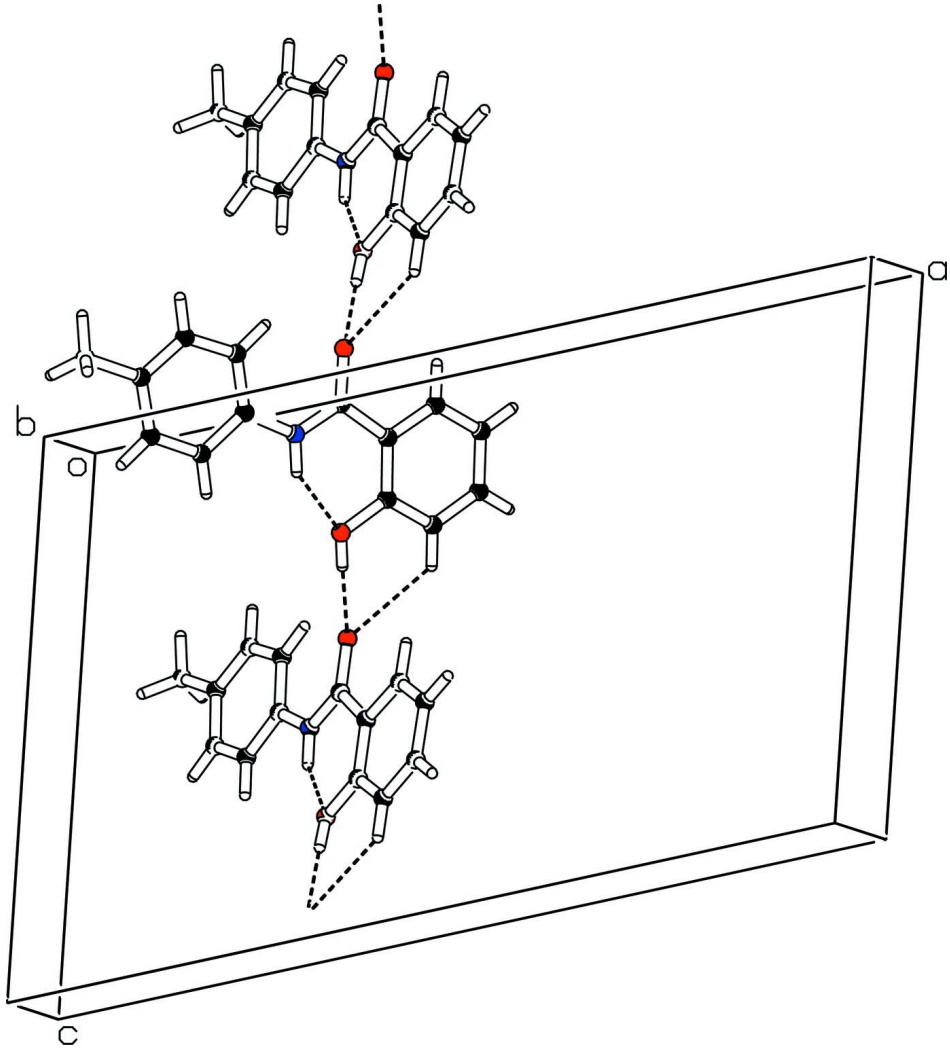

Figure 2

The partial packing diagram which shows that molecules form supramolecular chains extending along the *c*-axis. The dotted line indicate the intramolecular H-bonding.

2-Hydroxy-*N*-(4-methylphenyl)benzamide

Crystal data

$C_{14}H_{13}NO_2$
$M_r = 227.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 19.4067\ (17)$ Å
$b = 4.9122\ (5)$ Å
$c = 12.7261\ (11)$ Å
$\beta = 104.793\ (4)°$
$V = 1172.96\ (19)$ Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.287$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1243 reflections
$\theta = 1.1–27.9°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Needle, colorless
0.34 × 0.14 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.6 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.979, T_{max} = 0.988
10416 measured reflections
2771 independent reflections
1243 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.9°, θ_{min} = 1.1°
h = −25→25
k = −4→6
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.159
S = 0.96
2771 reflections
156 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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 esds 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}
O1	0.29367 (9)	−0.2157 (4)	0.22720 (13)	0.0599 (7)
O2	0.29429 (9)	−0.0348 (3)	−0.09273 (12)	0.0598 (7)
N1	0.24804 (9)	0.0722 (4)	0.04697 (14)	0.0438 (7)
C1	0.33925 (11)	−0.2782 (5)	0.07185 (18)	0.0407 (8)
C2	0.33876 (12)	−0.3489 (5)	0.17802 (18)	0.0438 (8)
C3	0.38382 (13)	−0.5515 (5)	0.2327 (2)	0.0516 (9)
C4	0.42941 (13)	−0.6849 (5)	0.1833 (2)	0.0596 (11)
C5	0.43143 (13)	−0.6168 (6)	0.0796 (2)	0.0615 (11)
C6	0.38654 (13)	−0.4161 (5)	0.0249 (2)	0.0539 (10)
C7	0.29213 (12)	−0.0712 (5)	0.00262 (18)	0.0416 (8)
C8	0.19724 (12)	0.2725 (5)	−0.00178 (18)	0.0428 (8)
C9	0.18909 (14)	0.3743 (5)	−0.1055 (2)	0.0564 (10)
C10	0.13704 (14)	0.5697 (6)	−0.1449 (2)	0.0605 (11)
C11	0.09251 (13)	0.6670 (5)	−0.0859 (2)	0.0544 (10)
C12	0.10233 (14)	0.5654 (5)	0.0186 (2)	0.0592 (10)
C13	0.15368 (13)	0.3727 (5)	0.06023 (19)	0.0524 (9)
C14	0.03636 (15)	0.8783 (5)	−0.1313 (2)	0.0751 (11)

H1	0.29314	−0.29364	0.28396	0.0899*
H1A	0.25091	0.03812	0.11424	0.0525*
H3	0.38315	−0.59736	0.30329	0.0619*
H4	0.45896	−0.82174	0.22036	0.0714*
H5	0.46273	−0.70494	0.04648	0.0739*
H6	0.38794	−0.37165	−0.04556	0.0647*
H9	0.21810	0.31275	−0.14848	0.0677*
H10	0.13229	0.63728	−0.21461	0.0726*
H12	0.07355	0.62883	0.06158	0.0711*
H13	0.15915	0.30919	0.13074	0.0628*
H14A	0.03008	0.89281	−0.20839	0.1127*
H14B	0.05114	1.05104	−0.09782	0.1127*
H14C	−0.00787	0.82537	−0.11655	0.1127*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0753 (12)	0.0677 (13)	0.0429 (11)	0.0164 (10)	0.0262 (9)	0.0130 (9)
O2	0.0889 (13)	0.0586 (13)	0.0371 (10)	0.0035 (10)	0.0256 (9)	0.0009 (8)
N1	0.0496 (12)	0.0504 (14)	0.0318 (10)	0.0029 (10)	0.0111 (9)	0.0039 (9)
C1	0.0437 (13)	0.0379 (15)	0.0409 (14)	−0.0064 (11)	0.0117 (11)	−0.0060 (11)
C2	0.0449 (14)	0.0444 (16)	0.0438 (14)	−0.0034 (12)	0.0147 (12)	−0.0036 (12)
C3	0.0500 (14)	0.0479 (18)	0.0534 (16)	−0.0010 (13)	0.0070 (12)	0.0053 (13)
C4	0.0506 (16)	0.0481 (19)	0.077 (2)	0.0041 (13)	0.0109 (15)	0.0031 (14)
C5	0.0525 (16)	0.061 (2)	0.076 (2)	0.0033 (15)	0.0257 (15)	−0.0090 (16)
C6	0.0557 (16)	0.0571 (19)	0.0522 (16)	−0.0014 (14)	0.0197 (13)	−0.0048 (14)
C7	0.0494 (14)	0.0400 (16)	0.0365 (14)	−0.0101 (12)	0.0132 (11)	−0.0050 (11)
C8	0.0474 (14)	0.0383 (15)	0.0400 (14)	−0.0038 (12)	0.0062 (11)	0.0006 (11)
C9	0.0608 (16)	0.0616 (19)	0.0465 (16)	−0.0014 (15)	0.0130 (13)	0.0051 (14)
C10	0.0673 (18)	0.056 (2)	0.0515 (17)	−0.0024 (15)	0.0028 (14)	0.0110 (14)
C11	0.0544 (16)	0.0360 (16)	0.0628 (19)	−0.0060 (13)	−0.0031 (14)	−0.0021 (13)
C12	0.0613 (17)	0.0524 (19)	0.0615 (18)	0.0060 (14)	0.0112 (14)	−0.0038 (14)
C13	0.0599 (16)	0.0563 (18)	0.0397 (14)	0.0043 (14)	0.0105 (12)	0.0046 (12)
C14	0.0718 (19)	0.0511 (19)	0.086 (2)	0.0023 (16)	−0.0097 (16)	0.0010 (16)

Geometric parameters (Å, º)

O1—C2	1.366 (3)	C10—C11	1.368 (4)
O2—C7	1.238 (3)	C11—C12	1.387 (3)
O1—H1	0.8200	C11—C14	1.509 (4)
N1—C7	1.339 (3)	C12—C13	1.379 (4)
N1—C8	1.419 (3)	C3—H3	0.9300
N1—H1A	0.8600	C4—H4	0.9300
C1—C7	1.495 (3)	C5—H5	0.9300
C1—C6	1.392 (3)	C6—H6	0.9300
C1—C2	1.397 (3)	C9—H9	0.9300
C2—C3	1.389 (3)	C10—H10	0.9300
C3—C4	1.375 (4)	C12—H12	0.9300

C4—C5	1.372 (4)	C13—H13	0.9300
C5—C6	1.381 (4)	C14—H14A	0.9600
C8—C13	1.386 (3)	C14—H14B	0.9600
C8—C9	1.382 (3)	C14—H14C	0.9600
C9—C10	1.391 (4)		

C2—O1—H1	109.00	C11—C12—C13	121.6 (2)
C7—N1—C8	128.90 (19)	C8—C13—C12	120.8 (2)
C8—N1—H1A	116.00	C2—C3—H3	120.00
C7—N1—H1A	116.00	C4—C3—H3	120.00
C2—C1—C6	117.5 (2)	C3—C4—H4	120.00
C2—C1—C7	125.8 (2)	C5—C4—H4	120.00
C6—C1—C7	116.7 (2)	C4—C5—H5	120.00
O1—C2—C3	120.6 (2)	C6—C5—H5	120.00
O1—C2—C1	119.2 (2)	C1—C6—H6	119.00
C1—C2—C3	120.3 (2)	C5—C6—H6	119.00
C2—C3—C4	120.6 (2)	C8—C9—H9	120.00
C3—C4—C5	120.2 (2)	C10—C9—H9	120.00
C4—C5—C6	119.3 (2)	C9—C10—H10	118.00
C1—C6—C5	122.1 (2)	C11—C10—H10	118.00
N1—C7—C1	118.03 (19)	C11—C12—H12	119.00
O2—C7—C1	120.5 (2)	C13—C12—H12	119.00
O2—C7—N1	121.5 (2)	C8—C13—H13	120.00
N1—C8—C9	124.5 (2)	C12—C13—H13	120.00
N1—C8—C13	117.0 (2)	C11—C14—H14A	109.00
C9—C8—C13	118.5 (2)	C11—C14—H14B	109.00
C8—C9—C10	119.3 (2)	C11—C14—H14C	109.00
C9—C10—C11	123.1 (2)	H14A—C14—H14B	109.00
C10—C11—C14	121.7 (2)	H14A—C14—H14C	109.00
C10—C11—C12	116.7 (2)	H14B—C14—H14C	109.00
C12—C11—C14	121.6 (2)		

C8—N1—C7—O2	2.0 (4)	C1—C2—C3—C4	0.0 (4)
C8—N1—C7—C1	−178.1 (2)	C2—C3—C4—C5	0.8 (4)
C7—N1—C8—C9	−6.3 (4)	C3—C4—C5—C6	−1.0 (4)
C7—N1—C8—C13	174.3 (2)	C4—C5—C6—C1	0.4 (4)
C6—C1—C2—O1	179.2 (2)	N1—C8—C9—C10	179.6 (2)
C6—C1—C2—C3	−0.5 (4)	C13—C8—C9—C10	−1.0 (4)
C7—C1—C2—O1	−2.3 (4)	N1—C8—C13—C12	−179.2 (2)
C7—C1—C2—C3	177.9 (2)	C9—C8—C13—C12	1.4 (4)
C2—C1—C6—C5	0.3 (4)	C8—C9—C10—C11	−0.4 (4)
C7—C1—C6—C5	−178.3 (2)	C9—C10—C11—C12	1.4 (4)
C2—C1—C7—O2	−176.0 (2)	C9—C10—C11—C14	−179.7 (2)
C2—C1—C7—N1	4.1 (4)	C10—C11—C12—C13	−1.0 (4)
C6—C1—C7—O2	2.5 (3)	C14—C11—C12—C13	−179.9 (2)
C6—C1—C7—N1	−177.5 (2)	C11—C12—C13—C8	−0.4 (4)
O1—C2—C3—C4	−179.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.78	2.596 (2)	179
N1—H1*A*···O1	0.86	1.92	2.647 (2)	141
C3—H3···O2^{i}	0.93	2.51	3.179 (3)	129
C9—H9···O2	0.93	2.25	2.840 (3)	121

Symmetry code: (i) x, $-y-1/2$, $z+1/2$.