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N-Benzyl-2-hydroxybenzamide

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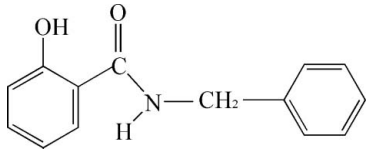
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 12.9.

In the title compound, $C_{14}H_{13}NO_2$, the mean planes through the benzyl and 2-hydoxybenzamide units make a dihedral angle of 68.81 (7)°. There is an intramolecular O—H···O hydrogen bond involving the carbonyl O atom and the 2-hydroxy substituent. In the crystal structure, N—H···O hydrogen bonds link symmetry-related molecules into one-dimensional chains extending along the *a*-axis direction. These chains are further connected *via* C—H···O hydrogen bonds, forming a sheet-like structure

Related literature

For related literature, see: Agwade (1982); Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Monoclinic, $P2_1/n$
a = 12.478 (3) Å
b = 8.3503 (17) Å
c = 12.664 (3) Å
β = 118.02 (3)°
V = 1164.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 290 (2) K
0.33 × 0.22 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.977, T_{max} = 0.983
11112 measured reflections
2665 independent reflections
1648 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 1.03
2665 reflections
207 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H*N*1···O1^{i}	0.882 (18)	2.083 (18)	2.9191 (18)	158.1 (18)
O1—H*O*1···O2	0.98 (3)	1.56 (3)	2.4886 (19)	157 (2)
C2—H2···O1^{i}	0.956 (19)	2.58 (2)	3.507 (2)	162.5 (15)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: SU2048).

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supplementary materials

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N-Benzyl-2-hydroxybenzamide

Q.-X. Zhang and B.-S. Zhang

Comment

Over a quater of a century ago (Agwade, 1982) published a thesis on Potential Central Nervous System Active Agents, which included the synthesis of aromatic *N*-benzyl amides. One of the compounds synthesized was N-benzyl-2-hydroxy-benzamide, (I), whose crystal structure has not been descibed until now.

The molecular structure of compound I is illustrated in Fig. 1. The bond lengths and angles are close to normal values (Allen *et al.*, 1987). There is an intramolecular O-H···O hydrogen bond in the molecule involving the carbonyl O-atom and the 2-hydroxyl substituent (Table 1). The best planes through the benzyl (atoms C8,C9-C14) and the 2-hydoxybenzamide (atoms C1-C6,C7,N1,O1,O2) moieties are inclined to one another by 68.81 (7)°.

In the crystal structure of I symmetry related molecules are connected via an N-H···O hydrogen bond to form chains running along the a direction. These chains are further connected connected via C-H···O hydrogen bonds (Table 1) to form a sheet-like structure (Fig 2).

Experimental

Freshly prepared $CuCO_3$ (0.310 g 2.50 mmol), $[C_6H_4(COOC_6H_4CONHCH_2ph)_2]$(0.350 g 0.601 mmol), 2-chloro-benzoic acid (0.160 g 1.022 mmol), and 15 ml CH_3OH/H_2O (1:2,*v*/*v*) were mixed and stirred for *ca*. 1.5 h. The resulting suspension was heated in a 23 ml Teflon-lined stainless steel autoclave at 373 K for 7 days. After the autoclave was cooled to room temperature, and colorless block-like crystals, suitable for X-ray analysis, were obtained.

Refinement

All of the H atoms were located in difference Fourier syntheses and were freely refined: O-H = 0.98 (3), N-H = 0.882 (18), and C-H = 0.94 (2) - 1.010 (16) Å.

Figures

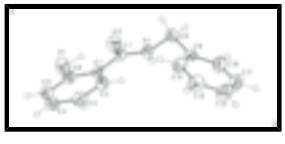

Fig. 1. A view of the moleculecular structure of I, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

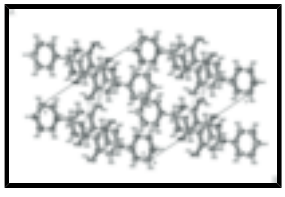

Fig. 2. The crystal packing diagram for compound I, viewed down the *b* axis. Dashed lines indicate N-H···O hydrogen bonds.

N-Benzyl-2-hydroxybenzamide

Crystal data

$C_{14}H_{13}NO_2$	F_{000} = 480
M_r = 227.25	D_x = 1.296 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6913 reflections
a = 12.478 (3) Å	θ = 3.0–27.5º
b = 8.3503 (17) Å	μ = 0.09 mm^{-1}
c = 12.664 (3) Å	T = 290 (2) K
β = 118.02 (3)º	Block, colorless
V = 1164.9 (6) Å^3	0.33 × 0.22 × 0.20 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	2665 independent reflections
Radiation source: fine-focus sealed tube	1648 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
Detector resolution: 10 pixels mm^{-1}	θ_{max} = 27.5º
T = 290(2) K	θ_{min} = 3.0º
ω scans	h = −15→16
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −10→10
T_{min} = 0.977, T_{max} = 0.983	l = −16→16
11112 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.0491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.116	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
2665 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
207 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: 0.011 (2)
Secondary atom site location: difference Fourier map	

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	0.29704 (10)	0.74227 (17)	−0.23736 (9)	0.0731 (4)
O2	0.49480 (9)	0.60089 (14)	−0.16419 (9)	0.0600 (4)
N1	0.64585 (9)	0.63326 (15)	0.02206 (11)	0.0449 (4)
C1	0.45255 (11)	0.76116 (16)	−0.03318 (11)	0.0396 (4)
C2	0.48553 (14)	0.82179 (19)	0.07995 (14)	0.0493 (5)
C3	0.40715 (15)	0.9140 (2)	0.10230 (16)	0.0592 (6)
C4	0.29300 (15)	0.9477 (2)	0.01061 (17)	0.0604 (6)
C5	0.25762 (14)	0.8909 (2)	−0.10172 (16)	0.0576 (6)
C6	0.33637 (12)	0.79771 (18)	−0.12499 (13)	0.0478 (5)
C7	0.53270 (11)	0.66022 (17)	−0.06264 (12)	0.0412 (4)
C8	0.73259 (14)	0.5375 (2)	0.00128 (16)	0.0508 (5)
C9	0.80422 (12)	0.63678 (17)	−0.04347 (14)	0.0460 (5)
C10	0.92320 (15)	0.6768 (3)	0.03099 (19)	0.0722 (7)
C11	0.98716 (18)	0.7699 (3)	−0.0108 (2)	0.0875 (9)
C12	0.9333 (2)	0.8228 (3)	−0.1254 (2)	0.0785 (9)
C13	0.81540 (19)	0.7850 (3)	−0.20000 (19)	0.0721 (8)
C14	0.75139 (16)	0.6917 (2)	−0.15893 (16)	0.0596 (6)
HN1	0.6728 (14)	0.6819 (19)	0.0917 (16)	0.059 (5)*
H2	0.5651 (15)	0.7995 (18)	0.1431 (15)	0.060 (5)*
HO1	0.367 (2)	0.681 (3)	−0.230 (2)	0.106 (7)*
H3	0.4331 (15)	0.952 (2)	0.1817 (17)	0.078 (5)*
H4	0.2386 (15)	1.009 (2)	0.0252 (15)	0.071 (5)*
H5	0.1770 (17)	0.913 (2)	−0.1697 (16)	0.081 (5)*
H8A	0.6833 (14)	0.455 (2)	−0.0610 (14)	0.062 (5)*
H8B	0.7896 (14)	0.4913 (19)	0.0805 (15)	0.062 (5)*
H10	0.9607 (17)	0.633 (2)	0.1088 (19)	0.087 (6)*
H11	1.070 (2)	0.793 (3)	0.042 (2)	0.107 (7)*
H12	0.9743 (19)	0.887 (3)	−0.1597 (18)	0.099 (7)*
H13	0.7716 (18)	0.825 (3)	−0.283 (2)	0.098 (7)*
H14	0.6696 (16)	0.668 (2)	−0.2122 (15)	0.070 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0512 (6)	0.1059 (10)	0.0395 (6)	0.0150 (7)	0.0024 (5)	−0.0056 (6)
O2	0.0503 (6)	0.0798 (8)	0.0421 (6)	0.0005 (5)	0.0152 (5)	−0.0147 (5)
N1	0.0376 (6)	0.0549 (8)	0.0399 (7)	0.0001 (5)	0.0162 (5)	0.0025 (6)
C1	0.0369 (6)	0.0420 (8)	0.0378 (7)	−0.0052 (6)	0.0159 (5)	0.0030 (6)
C2	0.0465 (8)	0.0557 (10)	0.0433 (8)	−0.0040 (7)	0.0190 (7)	−0.0014 (7)
C3	0.0664 (10)	0.0594 (10)	0.0604 (11)	−0.0070 (8)	0.0370 (9)	−0.0106 (8)
C4	0.0586 (10)	0.0493 (10)	0.0853 (13)	0.0013 (8)	0.0438 (9)	0.0000 (9)
C5	0.0440 (8)	0.0553 (10)	0.0696 (11)	0.0052 (7)	0.0235 (8)	0.0109 (8)
C6	0.0408 (7)	0.0533 (9)	0.0436 (8)	−0.0018 (7)	0.0150 (6)	0.0048 (7)
C7	0.0379 (7)	0.0458 (8)	0.0374 (8)	−0.0052 (6)	0.0156 (5)	0.0021 (6)
C8	0.0454 (8)	0.0501 (9)	0.0583 (10)	0.0065 (7)	0.0256 (7)	0.0099 (8)
C9	0.0447 (7)	0.0410 (8)	0.0558 (9)	0.0018 (6)	0.0266 (6)	−0.0020 (7)
C10	0.0477 (9)	0.0840 (14)	0.0753 (13)	−0.0025 (9)	0.0209 (8)	0.0173 (11)
C11	0.0510 (11)	0.0993 (17)	0.1074 (18)	−0.0151 (11)	0.0333 (11)	0.0117 (13)
C12	0.0808 (13)	0.0764 (14)	0.1031 (17)	−0.0141 (11)	0.0639 (13)	−0.0013 (12)
C13	0.0835 (13)	0.0814 (14)	0.0652 (12)	−0.0113 (10)	0.0464 (10)	0.0005 (10)
C14	0.0579 (10)	0.0695 (11)	0.0538 (10)	−0.0107 (8)	0.0283 (8)	−0.0039 (8)

Geometric parameters (Å, °)

O1—C6	1.3506 (18)	C10—C11	1.385 (3)
O2—C7	1.2456 (17)	C11—C12	1.355 (3)
O1—HO1	0.98 (3)	C12—C13	1.360 (4)
N1—C7	1.3311 (19)	C13—C14	1.381 (3)
N1—C8	1.466 (2)	C2—H2	0.956 (19)
N1—HN1	0.882 (18)	C3—H3	0.954 (19)
C1—C7	1.483 (2)	C4—H4	0.94 (2)
C1—C6	1.401 (2)	C5—H5	0.99 (2)
C1—C2	1.387 (2)	C8—H8A	1.010 (16)
C2—C3	1.375 (3)	C8—H8B	0.995 (17)
C3—C4	1.379 (3)	C10—H10	0.94 (2)
C4—C5	1.361 (3)	C11—H11	0.95 (3)
C5—C6	1.389 (3)	C12—H12	0.97 (3)
C8—C9	1.511 (3)	C13—H13	0.99 (2)
C9—C14	1.370 (2)	C14—H14	0.94 (2)
C9—C10	1.375 (3)		
O1···O2	2.4886 (19)	C9···H4^{iv}	3.034 (17)
O1···N1^{i}	2.9191 (18)	C14···H4^{iv}	2.989 (17)
O2···C14	3.260 (3)	HN1···C2	2.554 (19)
O2···O1	2.4886 (19)	HN1···H2	2.00 (3)
O1···H2^{i}	2.58 (2)	HN1···O1^{iii}	2.083 (18)
O1···HN1^{i}	2.083 (18)	H2···N1	2.597 (18)
O2···HO1	1.56 (3)	H2···HN1	2.00 (3)
O2···H8A	2.416 (18)	H2···O1^{iii}	2.58 (2)

O2···H14	2.59 (2)	HO1···O2	1.56 (3)
O2···H5^{ii}	2.692 (19)	HO1···C7	2.16 (2)
N1···O1^{iii}	2.9191 (18)	HO1···H5^{ii}	2.50 (3)
N1···H2	2.597 (18)	H4···C9^{iv}	3.034 (17)
C1···C3^{iv}	3.554 (2)	H4···C14^{iv}	2.989 (17)
C1···C8^{v}	3.549 (2)	H5···O2^{vi}	2.692 (19)
C3···C1^{iv}	3.554 (2)	H5···HO1^{vi}	2.50 (3)
C6···C8^{v}	3.507 (2)	H8A···O2	2.416 (18)
C7···C7^{v}	3.400 (2)	H8A···H14	2.56 (2)
C7···C14	3.483 (3)	H8A···H13^{vii}	2.54 (3)
C8···C1^{v}	3.549 (2)	H8A···C1^{v}	3.075 (18)
C8···C6^{v}	3.507 (2)	H8A···C2^{v}	3.060 (18)
C14···C7	3.483 (3)	H8B···H10	2.32 (3)
C14···O2	3.260 (3)	H8B···C6^{v}	3.073 (17)
C1···H8A^{v}	3.075 (18)	H10···H8B	2.32 (3)
C2···H8A^{v}	3.060 (18)	H13···H8A^{viii}	2.54 (3)
C2···HN1	2.554 (19)	H14···O2	2.59 (2)
C6···H8B^{v}	3.073 (17)	H14···C7	3.09 (2)
C7···H14	3.09 (2)	H14···H8A	2.56 (2)
C7···HO1	2.16 (2)		
C6—O1—HO1	102.3 (13)	C9—C14—C13	121.17 (19)
C7—N1—C8	122.74 (13)	C1—C2—H2	118.7 (11)
C7—N1—HN1	119.3 (12)	C3—C2—H2	119.8 (11)
C8—N1—HN1	117.7 (13)	C2—C3—H3	118.8 (12)
C6—C1—C7	118.17 (12)	C4—C3—H3	121.6 (12)
C2—C1—C6	117.83 (15)	C3—C4—H4	120.2 (11)
C2—C1—C7	124.00 (14)	C5—C4—H4	119.2 (11)
C1—C2—C3	121.50 (16)	C4—C5—H5	122.9 (12)
C2—C3—C4	119.62 (17)	C6—C5—H5	116.9 (12)
C3—C4—C5	120.55 (19)	N1—C8—H8A	106.4 (11)
C4—C5—C6	120.15 (17)	N1—C8—H8B	105.6 (11)
C1—C6—C5	120.35 (14)	C9—C8—H8A	109.4 (10)
O1—C6—C1	121.46 (15)	C9—C8—H8B	108.8 (11)
O1—C6—C5	118.19 (15)	H8A—C8—H8B	114.1 (13)
O2—C7—C1	120.79 (13)	C9—C10—H10	117.9 (14)
O2—C7—N1	120.61 (14)	C11—C10—H10	121.6 (14)
N1—C7—C1	118.60 (12)	C10—C11—H11	118.5 (15)
N1—C8—C9	112.64 (13)	C12—C11—H11	121.0 (15)
C8—C9—C10	120.97 (16)	C11—C12—H12	123.9 (13)
C8—C9—C14	120.74 (16)	C13—C12—H12	116.2 (13)
C10—C9—C14	118.28 (18)	C12—C13—H13	122.5 (15)
C9—C10—C11	120.3 (2)	C14—C13—H13	117.6 (15)
C10—C11—C12	120.5 (2)	C9—C14—H14	120.7 (11)
C11—C12—C13	119.9 (2)	C13—C14—H14	118.2 (11)
C12—C13—C14	119.8 (2)		

C8—N1—C7—O2	1.6 (2)	C2—C3—C4—C5	−0.2 (3)
C8—N1—C7—C1	−178.95 (14)	C3—C4—C5—C6	0.2 (3)
C7—N1—C8—C9	89.06 (18)	C4—C5—C6—O1	179.22 (16)
C6—C1—C2—C3	0.4 (2)	C4—C5—C6—C1	0.1 (2)
C7—C1—C2—C3	−179.59 (16)	N1—C8—C9—C10	104.4 (2)
C2—C1—C6—O1	−179.48 (15)	N1—C8—C9—C14	−74.4 (2)
C2—C1—C6—C5	−0.4 (2)	C8—C9—C10—C11	−179.0 (2)
C7—C1—C6—O1	0.5 (2)	C14—C9—C10—C11	−0.2 (3)
C7—C1—C6—C5	179.56 (15)	C8—C9—C14—C13	178.77 (18)
C2—C1—C7—O2	175.27 (15)	C10—C9—C14—C13	−0.1 (3)
C2—C1—C7—N1	−4.2 (2)	C9—C10—C11—C12	0.1 (4)
C6—C1—C7—O2	−4.7 (2)	C10—C11—C12—C13	0.3 (4)
C6—C1—C7—N1	175.80 (14)	C11—C12—C13—C14	−0.6 (4)
C1—C2—C3—C4	−0.1 (3)	C12—C13—C14—C9	0.5 (3)

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*−1/2; (ii) −*x*+1/2, *y*−1/2, −*z*−1/2; (iii) *x*+1/2, −*y*+3/2, *z*+1/2; (iv) −*x*+1, −*y*+2, −*z*; (v) −*x*+1, −*y*+1, −*z*; (vi) −*x*+1/2, *y*+1/2, −*z*−1/2; (vii) −*x*+3/2, *y*−1/2, −*z*−1/2; (viii) −*x*+3/2, *y*+1/2, −*z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—HN1···O1^{iii}	0.882 (18)	2.083 (18)	2.9191 (18)	158.1 (18)
O1—HO1···O2	0.98 (3)	1.56 (3)	2.4886 (19)	157 (2)
C2—H2···O1^{iii}	0.956 (19)	2.58 (2)	3.507 (2)	162.5 (15)
C14—H14···O2	0.94 (2)	2.59 (2)	3.260 (3)	128.8 (14)

Symmetry codes: (iii) *x*+1/2, −*y*+3/2, *z*+1/2.

Fig. 1

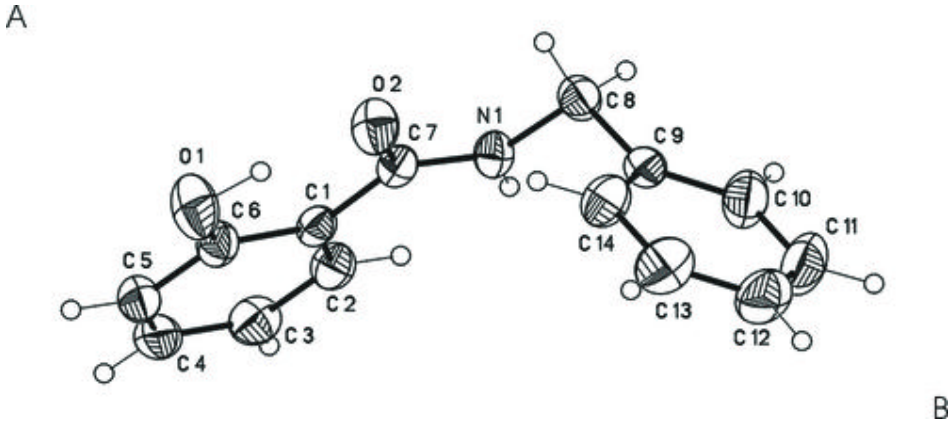

Fig. 2