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4-Hydroxybenzohydrazide

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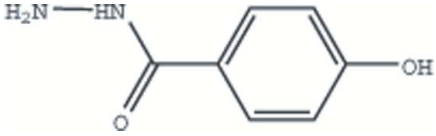
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.118; data-to-parameter ratio = 15.9.

In the title compound, $C_7H_8N_2O_2$, the mean planes of the benzene ring and the planar hydrazide group are inclined at 25.75 (6)° with respect to each other. The structure is stabilized by intermolecular N—H···O and O—H···N hydrogen bonds.

Related literature

For related structures see: Ashiq, Jamal *et al.* (2008, 2009); Hanif *et al.* (2007); Jamal *et al.* (2008); Kallel *et al.* (1992); Saraogi *et al.* (2002). For the biological activity of hydrazides, see: Ara *et al.* (2007); Ashiq, Ara *et al.* (2008); Maqsood *et al.* (2006).



Experimental

Crystal data

$C_7H_8N_2O_2$
M_r = 152.15
Monoclinic, $P2_1/c$
a = 5.0587 (2) Å
b = 17.2149 (9) Å
c = 7.8178 (5) Å
β = 93.489 (2)°
V = 679.55 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.32 × 0.18 × 0.12 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.965, T_{max} = 0.992
7324 measured reflections
1697 independent reflections
1348 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.118
S = 1.06
1697 reflections
107 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.13	2.9243 (14)	153
O1—H1A···N2^{ii}	0.82	1.98	2.7852 (16)	174
N2—H12···O1^{iii}	0.89 (2)	2.37 (2)	3.223 (2)	160
N2—H22···O2^{iv}	0.90 (2)	2.22 (2)	3.056 (2)	155

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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); 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: PV2171).

References

Ara, R., Ashiq, U., Mahroof-Tahir, M., Maqsood, Z. T., Khan, K. M., Lodhi, M. A. & Choudhary, M. I. (2007). *Chem. Biodivers.* **4**, 58–71.
Ashiq, U., Ara, R., Mahroof-Tahir, M., Maqsood, Z. T., Khan, K. M., Khan, S. N., Siddiqui, H. & Choudhary, M. I. (2008). *Chem. Biodivers.* **5**, 82–92.
Ashiq, U., Jamal, R. A., Mahroof-Tahir, M., Keramidas, A. D., Maqsood, Z. T., Khan, K. M. & Tahir, M. N. (2008). *Anal. Sci X*, **24**, 103–104.
Ashiq, U., Jamal, R. A., Tahir, M. N., Yousuf, S. & Khan, I. U. (2009). *Acta Cryst.* E**65**, o1551.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hanif, M., Qadeer, G., Rama, N. H., Rafiq, M. & Ružička, A. (2007). *Acta Cryst.* E**63**, o4829.
Jamal, R. A., Ashiq, U., Arshad, M. N., Maqsood, Z. T. & Khan, I. U. (2008). *Acta Cryst.* E**64**, o2188.
Kallel, A., Amor, B. H., Svoboda, I. & Fuess, H. (1992). *Z. Kristallogr.* **198**, 137–140.
Maqsood, Z. T., Khan, K. M., Ashiq, U., Jamal, R. A., Chohan, Z. H., Mahroof-Tahir, M. & Supuran, C. T. (2006). *J. Enz. Inhib. Med. Chem.* **21**, 37–42.
Saraogi, I., Mruthyunjayaswamy, B. H. M., Ijare, O. B., Jadegoud, Y. & Guru Row, T. N. (2002). *Acta Cryst.* E**58**, o1341–o1342.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o1764 [doi:10.1107/S1600536809025094]

4-Hydroxybenzohydrazide

Rifat Ara Jamal, Uzma Ashiq, Muhammad Nadeem Arshad, Zahida Tasneem Maqsood and Islam Ullah Khan

S1. Comment

Hydrazides are known to have different biological activities (Ashiq, Ara *et al.*, 2008; Ara *et al.*, 2007). In order to study the biological activity of 4-hydroxybenzohydrazide, we undertook the synthesis of the title compound, (I), and report its crystal structure in this paper. The title compound was found to be antifungal (Maqsood *et al.*, 2006). The crystal structures of benzhydrazide (Kallel *et al.*, 1992), *para*-chloro (Saraogi *et al.*, 2002), *para*-bromo (Ashiq, Jamal *et al.*, 2008), *para*-iodo (Jamal *et al.*, 2008) and *para*-methoxy (Ashiq, Jamal *et al.*, 2009) analogues of (I) have already been reported. The structure of (I) is isomorphous with its 3-hydroxy analogue (Hanif *et al.*, 2007).

The molecular structure of (I) has been presented in Fig. 1. The bond distances and bond angles in (I) are similar to the corresponding distances and angles reported in the structures quoted above. In (I), the mean-planes of the benzene ring (C1–C6) and planar hydrazide group (N1/N2/O2/C7) are inclined at 25.75 (6)° with respect to each other. The molecular packing diagram (Fig. 2) shows the presence of four intermolecular hydrogen bonds of the type N—H···O and O—H···N (details are given in Table 1).

S2. Experimental

All reagent-grade chemicals were obtained from Aldrich and Sigma Chemical companies and were used without further purification. To a solution of ethyl-4-hydroxybenzoate (3.32 g, 20 mmol) in 75 ml e thanol, hydrazine hydrate (5.0 ml, 100 mmol) was added. The mixture was refluxed for 5 h and a solid was obtained upon removal of the solvent by rotary evaporation. The resulting solid was washed with hexane to afford 4-hydroxybenzohydrazide (yield 65%) (Maqsood *et al.*, 2006).

S3. Refinement

H atoms were positioned geometrically, with aromatic C—H, O—H and N1—H1 distances 0.93, 0.82 and 0.86 Å, respectively, and constrained to ride on their parent atoms. The H-atoms attached to N2 atom were taken from Fourier synthesis and their coordinates were refined. The thermal parameter of H-atoms of was taken 1.2 times the equivalent isotropic displacement parameters of their parent C and N-atoms and 1.5 times the O-atom.

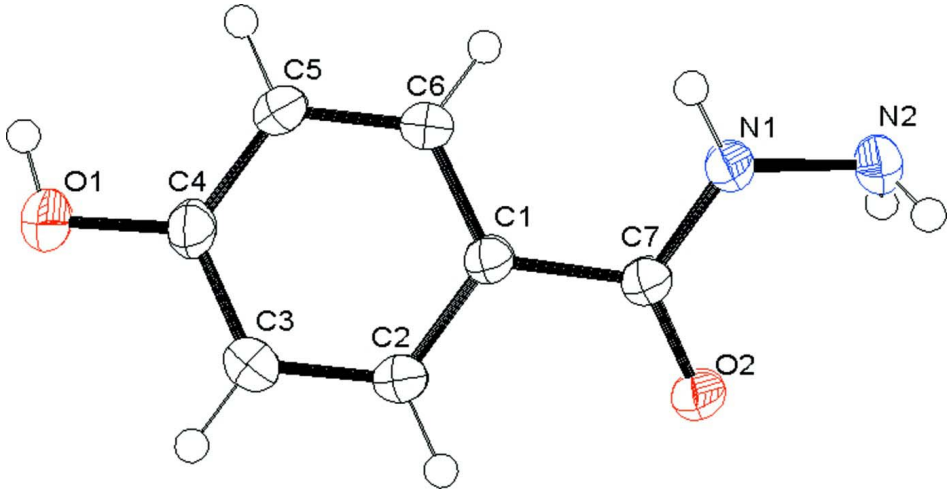

Figure 1

ORTEP plot of the title compound with the ellipsoids drawn at the 50% probability level.

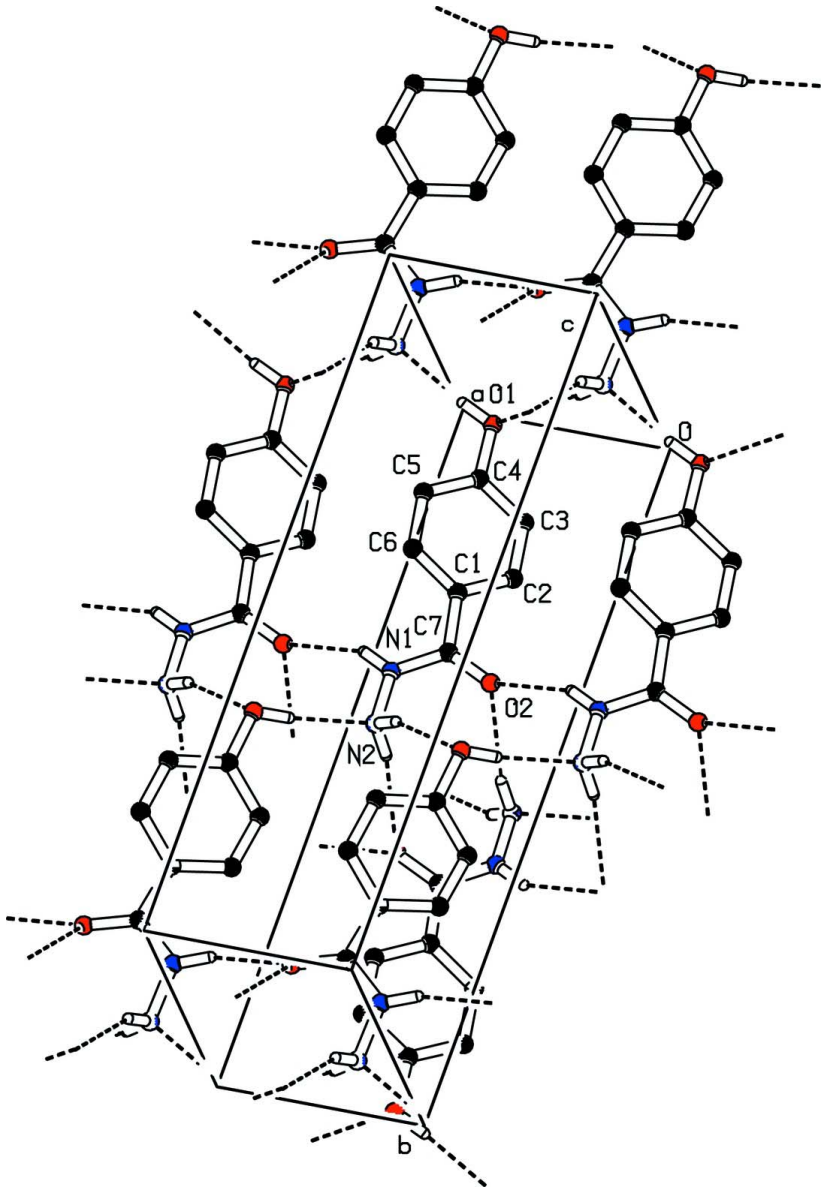

Figure 2

A packing diagram of (I). Hydrogen bonds are shown by dashed lines.

4-Hydroxybenzohydrazide

Crystal data

$C_7H_8N_2O_2$
$M_r = 152.15$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.0587\ (2)$ Å
$b = 17.2149\ (9)$ Å
$c = 7.8178\ (5)$ Å
$\beta = 93.489\ (2)°$
$V = 679.55\ (6)$ Å^3
$Z = 4$

$F(000) = 320$
$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2993 reflections
$\theta = 2.9–28.3°$
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Needle, colourless
0.32 × 0.18 × 0.12 mm

Data collection

Bruker Kappa APEX2 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.965, T_{max} = 0.992
7324 measured reflections
1697 independent reflections
1348 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 28.3°, θ_{min} = 2.4°
$h = -6 \rightarrow 6$
$k = -22 \rightarrow 23$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.118
S = 1.06
1697 reflections
107 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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.1539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7565 (2)	0.04052 (5)	0.14740 (17)	0.0478 (3)
H1A	0.8946	0.0291	0.2020	0.072*
O2	0.36833 (17)	0.38981 (5)	0.10180 (14)	0.0364 (3)
N1	0.8045 (2)	0.40995 (6)	0.15266 (16)	0.0331 (3)
H1	0.9606	0.3900	0.1554	0.040*
N2	0.7783 (2)	0.49074 (6)	0.1772 (2)	0.0381 (3)
H12	0.647 (4)	0.4969 (10)	0.247 (2)	0.046*
H22	0.736 (3)	0.5124 (10)	0.075 (2)	0.046*
C1	0.6499 (2)	0.27877 (7)	0.12927 (16)	0.0244 (3)
C2	0.4705 (2)	0.22850 (7)	0.04589 (17)	0.0299 (3)
H2	0.3217	0.2486	−0.0145	0.036*
C3	0.5095 (3)	0.14912 (8)	0.05121 (18)	0.0335 (3)
H3	0.3892	0.1161	−0.0066	0.040*
C4	0.7289 (3)	0.11891 (7)	0.14320 (18)	0.0304 (3)
C5	0.9081 (2)	0.16847 (7)	0.22869 (19)	0.0325 (3)

H5	1.0545	0.1484	0.2915	0.039*
C6	0.8685 (2)	0.24751 (7)	0.22038 (18)	0.0307 (3)
H6	0.9904	0.2805	0.2768	0.037*
C7	0.5947 (2)	0.36334 (7)	0.12527 (16)	0.0255 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0407 (6)	0.0216 (5)	0.0792 (9)	0.0012 (4)	−0.0124 (5)	0.0027 (5)
O2	0.0201 (4)	0.0278 (5)	0.0605 (7)	0.0024 (3)	−0.0032 (4)	0.0034 (4)
N1	0.0203 (5)	0.0213 (5)	0.0574 (7)	0.0009 (4)	−0.0008 (5)	−0.0007 (5)
N2	0.0305 (6)	0.0206 (5)	0.0627 (9)	−0.0015 (4)	−0.0020 (6)	0.0009 (5)
C1	0.0202 (5)	0.0231 (5)	0.0299 (6)	0.0007 (4)	0.0011 (4)	0.0016 (5)
C2	0.0238 (6)	0.0277 (6)	0.0372 (7)	−0.0002 (4)	−0.0061 (5)	0.0024 (5)
C3	0.0299 (6)	0.0277 (6)	0.0418 (8)	−0.0046 (5)	−0.0057 (5)	−0.0017 (5)
C4	0.0288 (6)	0.0208 (6)	0.0418 (7)	−0.0002 (5)	0.0037 (5)	0.0024 (5)
C5	0.0240 (6)	0.0274 (6)	0.0450 (8)	0.0033 (5)	−0.0061 (5)	0.0045 (5)
C6	0.0238 (6)	0.0266 (6)	0.0408 (7)	−0.0009 (5)	−0.0067 (5)	−0.0006 (5)
C7	0.0210 (5)	0.0241 (6)	0.0311 (6)	0.0011 (4)	0.0004 (4)	0.0013 (5)

Geometric parameters (Å, º)

O1—C4	1.3569 (14)	C1—C7	1.4824 (16)
O1—H1A	0.8200	C2—C3	1.3809 (17)
O2—C7	1.2356 (14)	C2—H2	0.9300
N1—C7	1.3376 (15)	C3—C4	1.3866 (18)
N1—N2	1.4113 (15)	C3—H3	0.9300
N1—H1	0.8600	C4—C5	1.3864 (18)
N2—H12	0.89 (2)	C5—C6	1.3762 (17)
N2—H22	0.90 (2)	C5—H5	0.9300
C1—C6	1.3870 (17)	C6—H6	0.9300
C1—C2	1.3876 (17)		
C4—O1—H1A	109.5	C2—C3—H3	120.2
C7—N1—N2	122.18 (10)	C4—C3—H3	120.2
C7—N1—H1	118.9	O1—C4—C5	122.50 (12)
N2—N1—H1	118.9	O1—C4—C3	117.60 (12)
N1—N2—H12	106.3 (11)	C5—C4—C3	119.90 (12)
N1—N2—H22	108.1 (11)	C6—C5—C4	119.78 (12)
H12—N2—H22	110.4 (17)	C6—C5—H5	120.1
C6—C1—C2	118.52 (11)	C4—C5—H5	120.1
C6—C1—C7	122.35 (11)	C5—C6—C1	121.13 (12)
C2—C1—C7	119.05 (11)	C5—C6—H6	119.4
C3—C2—C1	120.98 (12)	C1—C6—H6	119.4
C3—C2—H2	119.5	O2—C7—N1	121.45 (11)
C1—C2—H2	119.5	O2—C7—C1	122.48 (11)
C2—C3—C4	119.68 (12)	N1—C7—C1	116.04 (10)

C6—C1—C2—C3	−0.8 (2)	C2—C1—C6—C5	0.0 (2)
C7—C1—C2—C3	−177.79 (12)	C7—C1—C6—C5	176.81 (12)
C1—C2—C3—C4	1.0 (2)	N2—N1—C7—O2	7.9 (2)
C2—C3—C4—O1	178.80 (12)	N2—N1—C7—C1	−170.63 (12)
C2—C3—C4—C5	−0.2 (2)	C6—C1—C7—O2	−152.94 (13)
O1—C4—C5—C6	−179.61 (13)	C2—C1—C7—O2	23.90 (18)
C3—C4—C5—C6	−0.6 (2)	C6—C1—C7—N1	25.57 (18)
C4—C5—C6—C1	0.8 (2)	C2—C1—C7—N1	−157.60 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.13	2.9243 (14)	153
O1—H1*A*···N2^{ii}	0.82	1.98	2.7852 (16)	174
N2—H12···O1^{iii}	0.89 (2)	2.37 (2)	3.223 (2)	160
N2—H22···O2^{iv}	0.90 (2)	2.22 (2)	3.056 (2)	155

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