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4-Hydroxy-*N*′-(4-hydroxybenzoyl)benzohydrazide

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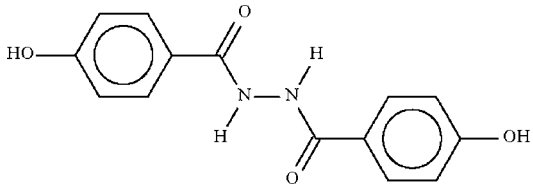
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.088; data-to-parameter ratio = 8.1.

In the molecule of the title compound, $C_{14}H_{12}N_2O_4$, the two benzene rings make a dihedral angle of 84.53 (8)°. O—H···O and N—H···O hydrogen bonds link adjacent molecules into a layer structure.

Related literature

For the unsubstituted parent compound, 1,2-dibenzoylhydrazine, see: Shanmuga Sundara Raj *et al.* (2000). For the 2-hydroxy substituted compound, 1,2-disalicyloylhydrazine, see: Chen *et al.* (2008).



Experimental

Crystal data

$C_{14}H_{12}N_2O_4$
M_r = 272.26
Orthorhombic, $P2_12_12_1$
a = 8.7058 (7) Å
b = 9.7646 (8) Å
c = 14.258 (1) Å
V = 1212.05 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 123 K
0.40 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
6928 measured reflections
1599 independent reflections
1475 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.088
S = 1.04
1599 reflections
197 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···O2^{i}	0.84 (1)	1.85 (1)	2.684 (2)	172 (3)
O4—H4o···O3^{ii}	0.85 (1)	1.83 (1)	2.675 (2)	178 (3)
N1—H1n···O2^{iii}	0.88 (1)	2.08 (1)	2.920 (2)	162 (2)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2507).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o969 [**doi:10.1107/S1600536809012136**]

4-Hydroxy-*N*'-(4-hydroxybenzoyl)benzohydrazide

K. M. Lo and S. W. Ng

Experimental

4-Hydroxybenzoylhydrazine (0.31 g, 2 mmol) and pyruvic acid (0.16 g, 2 mmol) were heated in ethanol (100 ml) for 3 h in an attemp to synthesize a Schiff base. Slow cooling of the filtered solution gave crystals of the hydrazide.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C). The amino and hydroxy H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and N–H 0.88±0.01 Å. Their temperature factors were refined.

Some 1159 Friedel pairs were merged.

Figures

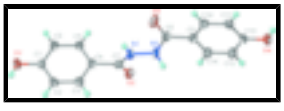

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{14}H_{12}N_2O_4$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

4-Hydroxy-*N*'-(4-hydroxybenzoyl)benzohydrazide

Crystal data

$C_{14}H_{12}N_2O_4$	F_{000} = 568
M_r = 272.26	D_x = 1.492 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3150 reflections
a = 8.7058 (7) Å	θ = 2.7–28.1º
b = 9.7646 (8) Å	μ = 0.11 mm^{-1}
c = 14.258 (1) Å	T = 123 K
V = 1212.05 (16) Å^3	Prism, light yellow
Z = 4	0.40 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer	1475 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.021
Monochromator: graphite	θ_{max} = 27.5º

T = 123 K	θ_{min} = 2.5º
ω scans	h = −7→11
Absorption correction: None	k = −12→12
6928 measured reflections	l = −18→18
1599 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.088	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.1781P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
1599 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
197 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.60946 (17)	0.59285 (14)	0.90517 (8)	0.0287 (3)
O2	0.72656 (15)	0.62247 (13)	0.46567 (8)	0.0247 (3)
O3	0.65093 (19)	0.92446 (15)	0.39648 (9)	0.0364 (4)
O4	0.63007 (17)	0.90074 (14)	−0.04878 (8)	0.0310 (3)
N1	0.49389 (17)	0.72003 (15)	0.47376 (9)	0.0217 (3)
N2	0.49553 (19)	0.74438 (15)	0.37802 (9)	0.0223 (3)
C1	0.6163 (2)	0.60858 (17)	0.81114 (11)	0.0206 (3)
C2	0.7010 (2)	0.52136 (18)	0.75329 (12)	0.0224 (4)
H2	0.7591	0.4487	0.7799	0.027*
C3	0.7002 (2)	0.54091 (17)	0.65708 (12)	0.0222 (4)
H3	0.7585	0.4818	0.6179	0.027*
C4	0.61465 (19)	0.64672 (17)	0.61727 (11)	0.0191 (3)
C5	0.5318 (2)	0.73400 (18)	0.67564 (11)	0.0214 (3)
H5	0.4735	0.8065	0.6491	0.026*
C6	0.5334 (2)	0.71626 (18)	0.77205 (11)	0.0235 (4)
H6	0.4781	0.7774	0.8114	0.028*
C7	0.6172 (2)	0.66161 (17)	0.51417 (11)	0.0197 (3)
C8	0.5846 (2)	0.84605 (18)	0.34327 (12)	0.0226 (4)
C9	0.5944 (2)	0.85689 (17)	0.23956 (12)	0.0210 (4)
C10	0.7023 (2)	0.94658 (17)	0.20197 (12)	0.0224 (4)
H10	0.7664	0.9979	0.2429	0.027*
C11	0.7180 (2)	0.96226 (18)	0.10568 (12)	0.0233 (4)
H11	0.7928	1.0232	0.0809	0.028*

C12	0.6230 (2)	0.88771 (17)	0.04537 (11)	0.0222 (4)
C13	0.5156 (2)	0.79694 (19)	0.08191 (11)	0.0265 (4)
H13	0.4517	0.7455	0.0409	0.032*
C14	0.5017 (2)	0.78146 (18)	0.17811 (12)	0.0247 (4)
H14	0.4285	0.7189	0.2027	0.030*
H1O	0.668 (3)	0.529 (2)	0.9222 (17)	0.045 (7)*
H4O	0.698 (2)	0.958 (2)	−0.0659 (18)	0.050 (8)*
H1N	0.4167 (19)	0.757 (2)	0.5039 (15)	0.031 (6)*
H2N	0.467 (3)	0.6748 (17)	0.3437 (14)	0.046 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0391 (8)	0.0299 (7)	0.0172 (6)	0.0076 (6)	−0.0011 (5)	0.0049 (5)
O2	0.0253 (6)	0.0290 (6)	0.0199 (5)	0.0028 (6)	0.0036 (5)	−0.0039 (5)
O3	0.0500 (9)	0.0399 (8)	0.0194 (6)	−0.0174 (7)	−0.0003 (6)	−0.0066 (6)
O4	0.0440 (9)	0.0313 (7)	0.0179 (6)	−0.0098 (7)	0.0005 (6)	0.0030 (5)
N1	0.0219 (7)	0.0300 (7)	0.0132 (6)	0.0027 (7)	0.0014 (6)	−0.0001 (6)
N2	0.0265 (8)	0.0276 (7)	0.0128 (6)	−0.0014 (7)	−0.0012 (6)	−0.0004 (5)
C1	0.0244 (9)	0.0209 (7)	0.0167 (7)	−0.0032 (7)	−0.0023 (6)	0.0014 (6)
C2	0.0238 (9)	0.0207 (7)	0.0227 (8)	0.0008 (7)	−0.0022 (7)	0.0036 (6)
C3	0.0216 (9)	0.0221 (8)	0.0230 (8)	0.0012 (7)	0.0014 (7)	−0.0016 (6)
C4	0.0192 (8)	0.0208 (7)	0.0173 (7)	−0.0039 (7)	−0.0004 (6)	0.0002 (6)
C5	0.0236 (9)	0.0206 (7)	0.0199 (7)	0.0021 (7)	−0.0005 (7)	0.0008 (6)
C6	0.0283 (9)	0.0236 (8)	0.0186 (8)	0.0026 (8)	0.0019 (7)	−0.0018 (7)
C7	0.0208 (8)	0.0188 (7)	0.0194 (8)	−0.0029 (7)	0.0009 (6)	−0.0025 (6)
C8	0.0231 (9)	0.0247 (8)	0.0201 (8)	0.0015 (7)	0.0006 (7)	−0.0026 (7)
C9	0.0231 (8)	0.0217 (8)	0.0181 (8)	0.0019 (7)	−0.0001 (6)	−0.0009 (6)
C10	0.0230 (9)	0.0217 (8)	0.0224 (8)	−0.0009 (7)	−0.0038 (7)	−0.0022 (6)
C11	0.0262 (9)	0.0210 (8)	0.0227 (8)	−0.0018 (7)	−0.0007 (7)	0.0027 (7)
C12	0.0282 (9)	0.0219 (8)	0.0166 (8)	0.0012 (8)	−0.0005 (6)	0.0014 (6)
C13	0.0296 (10)	0.0295 (9)	0.0206 (8)	−0.0065 (8)	−0.0028 (7)	−0.0026 (7)
C14	0.0267 (9)	0.0268 (8)	0.0206 (8)	−0.0064 (8)	0.0011 (7)	−0.0005 (7)

Geometric parameters (Å, °)

O1—C1	1.3506 (19)	C7—N1	1.345 (2)
O1—H1O	0.839 (10)	C8—N2	1.354 (2)
O2—C7	1.237 (2)	C8—C9	1.485 (2)
O3—C8	1.223 (2)	C9—C10	1.392 (2)
O4—C12	1.3497 (19)	C9—C14	1.400 (2)
O4—H4O	0.846 (10)	C10—C11	1.388 (2)
C1—C6	1.392 (2)	C10—H10	0.9500
C1—C2	1.396 (2)	C11—C12	1.398 (2)
C2—C3	1.385 (2)	C11—H11	0.9500
C2—H2	0.9500	C12—C13	1.390 (2)
C3—C4	1.395 (2)	C13—C14	1.385 (2)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.393 (2)	C14—H14	0.9500

C4—C7	1.477 (2)	N1—N2	1.3856 (18)
C5—C6	1.386 (2)	N1—H1N	0.877 (10)
C5—H5	0.9500	N2—H2N	0.874 (10)
C6—H6	0.9500		
C1—O1—H1O	110.1 (18)	N2—C8—C9	116.72 (15)
C12—O4—H4O	112.4 (19)	C10—C9—C14	118.62 (15)
O1—C1—C6	117.41 (15)	C10—C9—C8	117.85 (15)
O1—C1—C2	122.70 (15)	C14—C9—C8	123.53 (16)
C6—C1—C2	119.88 (15)	C11—C10—C9	121.10 (16)
C3—C2—C1	119.90 (16)	C11—C10—H10	119.5
C3—C2—H2	120.1	C9—C10—H10	119.5
C1—C2—H2	120.1	C10—C11—C12	119.54 (17)
C2—C3—C4	120.52 (16)	C10—C11—H11	120.2
C2—C3—H3	119.7	C12—C11—H11	120.2
C4—C3—H3	119.7	O4—C12—C13	117.63 (15)
C5—C4—C3	119.15 (15)	O4—C12—C11	122.39 (16)
C5—C4—C7	122.84 (15)	C13—C12—C11	119.98 (15)
C3—C4—C7	118.02 (15)	C14—C13—C12	119.96 (16)
C6—C5—C4	120.74 (16)	C14—C13—H13	120.0
C6—C5—H5	119.6	C12—C13—H13	120.0
C4—C5—H5	119.6	C13—C14—C9	120.80 (17)
C5—C6—C1	119.80 (16)	C13—C14—H14	119.6
C5—C6—H6	120.1	C9—C14—H14	119.6
C1—C6—H6	120.1	C7—N1—N2	119.10 (14)
O2—C7—N1	120.37 (14)	C7—N1—H1N	125.3 (15)
O2—C7—C4	122.52 (15)	N2—N1—H1N	114.8 (16)
N1—C7—C4	117.11 (14)	C8—N2—N1	119.49 (14)
O3—C8—N2	120.18 (16)	C8—N2—H2N	121.9 (16)
O3—C8—C9	123.09 (17)	N1—N2—H2N	114.5 (16)
O1—C1—C2—C3	178.36 (16)	N2—C8—C9—C14	9.1 (3)
C6—C1—C2—C3	−1.0 (3)	C14—C9—C10—C11	0.4 (3)
C1—C2—C3—C4	−0.4 (3)	C8—C9—C10—C11	−179.92 (17)
C2—C3—C4—C5	1.0 (3)	C9—C10—C11—C12	0.6 (3)
C2—C3—C4—C7	−179.43 (16)	C10—C11—C12—O4	178.43 (16)
C3—C4—C5—C6	−0.2 (3)	C10—C11—C12—C13	−1.1 (3)
C7—C4—C5—C6	−179.74 (16)	O4—C12—C13—C14	−178.89 (17)
C4—C5—C6—C1	−1.2 (3)	C11—C12—C13—C14	0.6 (3)
O1—C1—C6—C5	−177.59 (17)	C12—C13—C14—C9	0.3 (3)
C2—C1—C6—C5	1.8 (3)	C10—C9—C14—C13	−0.9 (3)
C5—C4—C7—O2	152.83 (17)	C8—C9—C14—C13	179.49 (17)
C3—C4—C7—O2	−26.7 (2)	O2—C7—N1—N2	−4.4 (2)
C5—C4—C7—N1	−27.4 (2)	C4—C7—N1—N2	175.75 (14)
C3—C4—C7—N1	153.10 (16)	O3—C8—N2—N1	−7.3 (3)
O3—C8—C9—C10	10.2 (3)	C9—C8—N2—N1	173.48 (15)
N2—C8—C9—C10	−170.57 (16)	C7—N1—N2—C8	−72.5 (2)
O3—C8—C9—C14	−170.11 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···O2^{i}	0.84 (1)	1.85 (1)	2.684 (2)	172 (3)
O4—H4o···O3^{ii}	0.85 (1)	1.83 (1)	2.675 (2)	178 (3)
N1—H1n···O2^{iii}	0.88 (1)	2.08 (1)	2.920 (2)	162 (2)

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

Fig. 1