Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Kong Mun Lo and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

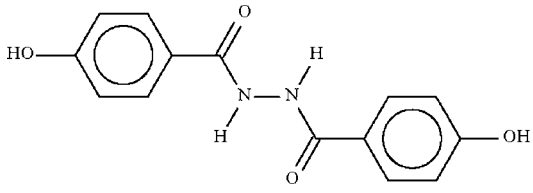
Received 31 March 2009; accepted 1 April 2009

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).

We thank the University of Malaya (FS339/2008 A) for supporting this study.

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

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Y.-T., Li, D.-C., Wang, D.-Q. & Zhu, Y.-H. (2008). *Acta Cryst.* E**64**, o120.
Shanmuga Sundara Raj, S., Yamin, B. M., Boshaala, A. M. A., Tarafder, M. T. H., Crouse, K. A. & Fun, H.-K. (2000). *Acta Cryst.* C**56**, 1011–1012.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

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

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

Kong Mun Lo and Seik Weng Ng

S1. 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.

S2. 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 1.2*U*(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.

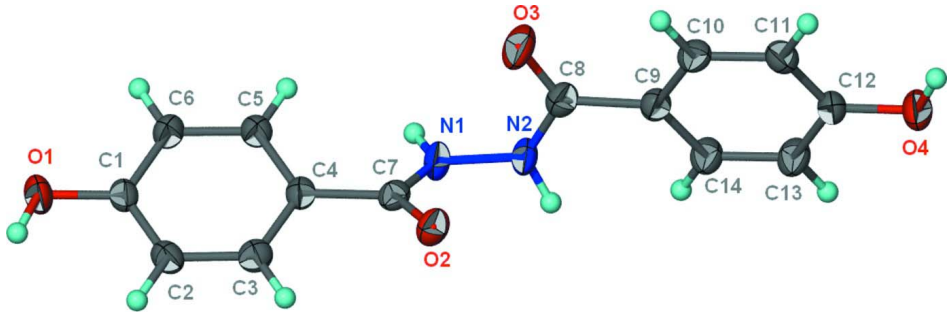


Figure 1

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

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

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6928 measured reflections
1599 independent reflections
1475 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
$h = -7 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.088$
$S = 1.04$
1599 reflections
197 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.1781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	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 (Å²)

	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, º)

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, º)

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) $x-1/2, -y+3/2, -z+1$.