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N,*N*′-Bis(4-hydroxybenzylidene)-hydrazine

Gang Liu, Ling Xie, Yan Wang* and Ji-De Wang

Department of Chemistry and Chemistry Engineering, Xinjiang University, Urumqi 830046, People's Republic of China
Correspondence e-mail: awangjd@xju.edu.cn

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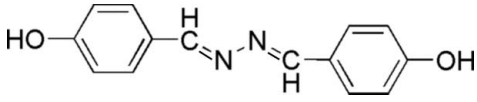
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.147; data-to-parameter ratio = 16.2.

The crystal structure of the title compound, $C_{14}H_{12}N_2O_2$, is stabilized by intermolecular hydrogen-bonding interactions.

Related literature

For related literature, see: Buu-Hoi *et al.*, (1953); Lal *et al.* (1997); Singh *et al.* (1982); Xu *et al.* (1994); Zheng *et al.* (2005).



Experimental

Crystal data

$C_{14}H_{12}N_2O_2$
M_r = 240.26
Monoclinic, $P2_1/c$
a = 12.587 (3) Å
b = 8.5349 (17) Å
c = 11.897 (2) Å
β = 114.12 (3)°
V = 1166.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
0.34 × 0.33 × 0.03 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.969, T_{max} = 0.997
10931 measured reflections
2663 independent reflections
2075 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.147
S = 1.01
2663 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···H2*O*^{i}	0.84 (10)	1.11 (10)	1.9303 (16)	163 (1)
O1—H1*O*···O2^{i}	0.84 (10)	1.94 (10)	2.7679 (16)	169 (1)
O2—H2*O*···H1*O*^{ii}	0.84 (10)	1.11 (10)	1.9393 (15)	168 (1)
O2—H2*O*···O1^{ii}	0.84 (10)	1.93 (10)	2.7679 (16)	175 (1)

Symmetry codes: (i) $x+1, y+1, z+1$; (ii) $x-1, y-1, z-1$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2274).

References

Buu-Hoi, N. P., Huong, N. D., Ham, N. H., Binon, F. & Royer, R. (1953). *J. Chem. Soc.* pp. 1358–1364.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Lal, R. A., Adhikari, S. & Pal, A. (1997). *J. Chem. Res.* **4**, 122–125.
Rigaku (2004). *RAPID-AUTO*. Version 3.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Singh, R. B., Jain, P. & Singh, R. P. (1982). *Talanta*, **29**, 77–82.
Xu, X.-X., You, X.-Z., Sun, Z.-F., Wang, X. & Liu, H.-X. (1994). *Acta Cryst.* C**50**, 1169–1171.
Zheng, P.-W., Wang, W. & Duan, X.-M. (2005). *Acta Cryst.* E**61**, o3020–o3021.

supplementary materials

Acta Cryst. (2007). E**63**, o2611 [**doi:10.1107/S1600536807018855**]

N,*N*'-Bis(4-hydroxybenzylidene)hydrazine

G. Liu, L. Xie, Y. Wang and J.-D. Wang

Comment

Acylhydrazones have been extensively investigated in recent years, as they are associated with various biological activities (Buu-Hoi *et al.*,1953). Furthermore, it also has interesting analytical properties (Singh *et al.*, 1982) and can be used as ligands in orgamometallic catalysts (Lal *et al.*, 1997). 2,2'-Azinodi-2-hydroxytoluene and *N*,*N*'-bis(4-chlorobenzylidene)hydrazine have been reported by Xu *et al.*, 1994 and Zheng *et al.*, 2005, respectively.

The molecular structure of the title compound (Fig. 1) contains intermolecular hydrogen bond [O1—H1O···O2 = 2.7302 (16) Å](Table 2), leading to an one-dimensional chain. Interesting another chain was hydrogen-bonded reversely to the chain through the other type of intermolecular hydrogen bond [O1—H10···N1 = 2.7590 (14) Å]. Thus, the structure can be attributted to a two dimensional framework (Fig.2). Two types of hydrogen bonds make the structure stabilize.

Experimental

The mixture of 4-hydroxybenzaldehyde (0.244 g) in 20 ml me thanol and hydrazine (0.146 g) in 40 ml me thanol was stirred 2 h with refluxing. The yellow produce was isolated by filtration, washed with diethyl ether and dried at room temperature for a yield of 0.15 g (53%). Analysis found (calculated) for the title compound (%): C 69.51(69.99); H 4.72(5.03); N 10.93 (11.66); O 14.84(13.32).

Refinement

The H atoms attached to the parent C were geometrically fixed with, and were treated as riding atoms, whereas the H atoms attached to the parent O atom were located from difference maps and were refined freely. The H atoms were positioned geometrically, with C—H = 0.95 - 0.99 Å, and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

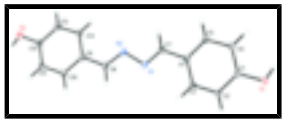

Fig. 1. A view of the molecule of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

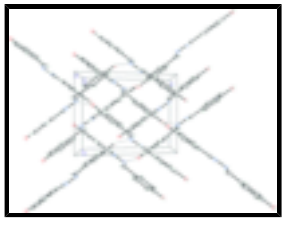

Fig. 2. The packing structure of the title compound viewed down the a-axis showing the molecular.

N,*N*'-Bis(4-Hydroxybenzylidene)hydrazine

Crystal data

$C_{14}H_{12}N_2O_2$	F_{000} = 504
M_r = 240.26	D_x = 1.368 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 528 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.587 (3) Å	Cell parameters from 8183 reflections
b = 8.5349 (17) Å	θ = 3.0–27.5º
c = 11.897 (2) Å	μ = 0.09 mm^{-1}
β = 114.12 (3)º	T = 153 (2) K
V = 1166.6 (4) Å^3	Chip, colourless
Z = 4	0.34 × 0.33 × 0.03 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer	2663 independent reflections
Radiation source: fine-focus sealed tube	2075 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 153(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.0º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −16→16
T_{min} = 0.969, T_{max} = 0.997	k = −10→11
10931 measured reflections	l = −15→15

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0904P)^2 + 0.38P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$(\Delta/\sigma)_{max}$ = 0.009
$wR(F^2)$ = 0.147	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
2663 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
164 parameters	Extinction coefficient: 0.010 (3)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

- 1.0038 (0.0089) x - 6.8322 (0.0048) y + 6.8379 (0.0074) z = 1.7177 (0.0012)

* 0.0000 (0.0011) C9 * 0.0033 (0.0011) C10 * -0.0039 (0.0011) C11 * 0.0012 (0.0011) C12 * 0.0022 (0.0012) C13 * -0.0028 (0.0011) C14

Rms deviation of fitted atoms = 0.0026

1.7154 (0.0212) x - 6.9219 (0.0065) y + 5.5155 (0.0214) z = 1.9752 (0.0035)

Angle to previous plane (with approximate esd) = 12.50 (0.18)

* -0.0847 (0.0007) C7 * -0.0854 (0.0007) C8 * 0.0845 (0.0007) N1 * 0.0856 (0.0007) N2

Rms deviation of fitted atoms = 0.0850

1.6200 (0.0080) x - 6.7985 (0.0046) y + 5.7888 (0.0069) z = 1.9768 (0.0052)

Angle to previous plane (with approximate esd) = 1.56 (0.19)

* 0.0152 (0.0010) C1 * -0.0105 (0.0010) C2 * -0.0041 (0.0010) C3 * 0.0141 (0.0010) C4 * -0.0097 (0.0010) C5 * -0.0049 (0.0010) C6

Rms deviation of fitted atoms = 0.0106

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.72875 (8)	0.61870 (12)	0.87357 (10)	0.0250 (3)
H1O	0.7962	0.6248	0.8759	0.038*
O2	−0.04201 (10)	−0.33486 (15)	−0.09068 (12)	0.0354 (3)
H2O	−0.1107	−0.3454	−0.0975	0.053*
N1	0.36829 (10)	0.16168 (14)	0.46180 (12)	0.0218 (3)
N2	0.32543 (10)	0.06609 (15)	0.35537 (12)	0.0237 (3)
C1	0.66180 (12)	0.52650 (16)	0.77724 (13)	0.0205 (3)
C2	0.54791 (11)	0.48685 (16)	0.75810 (13)	0.0206 (3)
H2	0.5150	0.5274	0.8111	0.025*
C3	0.48322 (12)	0.38881 (16)	0.66218 (14)	0.0210 (3)

H3	0.4062	0.3614	0.6502	0.025*
C4	0.52981 (12)	0.32924 (16)	0.58232 (13)	0.0205 (3)
C5	0.64248 (12)	0.37493 (17)	0.60033 (14)	0.0235 (3)
H5	0.6743	0.3385	0.5452	0.028*
C6	0.70851 (12)	0.47210 (18)	0.69680 (14)	0.0244 (3)
H6	0.7850	0.5014	0.7080	0.029*
C7	0.46655 (12)	0.22489 (16)	0.47989 (14)	0.0222 (3)
H7	0.4999	0.2022	0.4231	0.027*
C8	0.21725 (12)	0.03528 (17)	0.31936 (14)	0.0229 (3)
H8	0.1770	0.0776	0.3647	0.028*
C9	0.15253 (12)	−0.06125 (17)	0.21241 (14)	0.0225 (3)
C10	0.03306 (13)	−0.07915 (18)	0.17746 (15)	0.0261 (3)
H10	−0.0030	−0.0285	0.2239	0.031*
C11	−0.03409 (12)	−0.16936 (18)	0.07641 (15)	0.0267 (4)
H11	−0.1155	−0.1793	0.0533	0.032*
C12	0.01847 (13)	−0.24519 (18)	0.00911 (14)	0.0249 (3)
C13	0.13789 (13)	−0.22885 (19)	0.04311 (15)	0.0281 (4)
H13	0.1738	−0.2808	−0.0029	0.034*
C14	0.20428 (12)	−0.13778 (18)	0.14312 (15)	0.0255 (3)
H14	0.2855	−0.1269	0.1652	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0173 (5)	0.0312 (6)	0.0239 (6)	−0.0057 (4)	0.0056 (4)	−0.0074 (4)
O2	0.0274 (6)	0.0478 (7)	0.0314 (7)	−0.0141 (5)	0.0123 (5)	−0.0180 (5)
N1	0.0228 (6)	0.0218 (6)	0.0169 (6)	−0.0009 (5)	0.0044 (5)	−0.0021 (5)
N2	0.0253 (6)	0.0251 (6)	0.0188 (6)	−0.0023 (5)	0.0070 (5)	−0.0035 (5)
C1	0.0201 (6)	0.0192 (6)	0.0195 (7)	−0.0004 (5)	0.0055 (5)	−0.0003 (5)
C2	0.0199 (6)	0.0216 (7)	0.0213 (7)	−0.0008 (5)	0.0093 (5)	−0.0009 (5)
C3	0.0186 (6)	0.0218 (7)	0.0221 (7)	−0.0021 (5)	0.0081 (5)	0.0000 (5)
C4	0.0219 (6)	0.0199 (7)	0.0184 (7)	−0.0002 (5)	0.0070 (5)	0.0007 (5)
C5	0.0227 (7)	0.0271 (7)	0.0225 (8)	0.0020 (5)	0.0110 (6)	−0.0010 (6)
C6	0.0178 (6)	0.0293 (8)	0.0260 (8)	−0.0024 (5)	0.0088 (6)	−0.0012 (6)
C7	0.0239 (7)	0.0231 (7)	0.0189 (7)	0.0013 (5)	0.0082 (6)	0.0002 (5)
C8	0.0235 (7)	0.0247 (7)	0.0195 (7)	−0.0002 (5)	0.0076 (6)	−0.0015 (6)
C9	0.0227 (7)	0.0235 (7)	0.0196 (7)	−0.0026 (5)	0.0069 (5)	0.0001 (6)
C10	0.0246 (7)	0.0304 (8)	0.0250 (8)	−0.0023 (6)	0.0119 (6)	−0.0038 (6)
C11	0.0203 (7)	0.0324 (8)	0.0268 (8)	−0.0056 (6)	0.0092 (6)	−0.0028 (6)
C12	0.0260 (7)	0.0270 (7)	0.0205 (7)	−0.0073 (6)	0.0082 (6)	−0.0036 (6)
C13	0.0254 (7)	0.0329 (8)	0.0276 (8)	−0.0036 (6)	0.0125 (6)	−0.0077 (6)
C14	0.0199 (6)	0.0293 (8)	0.0265 (8)	−0.0030 (5)	0.0086 (6)	−0.0039 (6)

Geometric parameters (Å, °)

O1—C1	1.3615 (17)	C5—H5	0.9500
O1—H1O	0.8400	C6—H6	0.9500
O2—C12	1.3550 (19)	C7—H7	0.9500
O2—H2O	0.8400	C8—C9	1.454 (2)

N1—C7	1.2843 (19)	C8—H8	0.9500
N1—N2	1.4148 (17)	C9—C10	1.395 (2)
N2—C8	1.2767 (19)	C9—C14	1.403 (2)
C1—C6	1.392 (2)	C10—C11	1.386 (2)
C1—C2	1.3982 (18)	C10—H10	0.9500
C2—C3	1.3806 (19)	C11—C12	1.390 (2)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.400 (2)	C12—C13	1.395 (2)
C3—H3	0.9500	C13—C14	1.380 (2)
C4—C5	1.400 (2)	C13—H13	0.9500
C4—C7	1.456 (2)	C14—H14	0.9500
C5—C6	1.384 (2)		
C1—O1—H1O	109.5	N1—C7—H7	118.1
C12—O2—H2O	109.5	C4—C7—H7	118.1
C7—N1—N2	112.40 (13)	N2—C8—C9	123.35 (14)
C8—N2—N1	112.55 (13)	N2—C8—H8	118.3
O1—C1—C6	118.79 (12)	C9—C8—H8	118.3
O1—C1—C2	121.18 (13)	C10—C9—C14	118.45 (14)
C6—C1—C2	120.02 (13)	C10—C9—C8	118.23 (14)
C3—C2—C1	120.03 (13)	C14—C9—C8	123.31 (13)
C3—C2—H2	120.0	C11—C10—C9	121.35 (14)
C1—C2—H2	120.0	C11—C10—H10	119.3
C2—C3—C4	120.79 (12)	C9—C10—H10	119.3
C2—C3—H3	119.6	C10—C11—C12	119.55 (13)
C4—C3—H3	119.6	C10—C11—H11	120.2
C3—C4—C5	118.28 (13)	C12—C11—H11	120.2
C3—C4—C7	123.55 (13)	O2—C12—C11	122.59 (13)
C5—C4—C7	118.16 (13)	O2—C12—C13	117.62 (14)
C6—C5—C4	121.41 (14)	C11—C12—C13	119.78 (14)
C6—C5—H5	119.3	C14—C13—C12	120.49 (14)
C4—C5—H5	119.3	C14—C13—H13	119.8
C5—C6—C1	119.39 (13)	C12—C13—H13	119.8
C5—C6—H6	120.3	C13—C14—C9	120.37 (13)
C1—C6—H6	120.3	C13—C14—H14	119.8
N1—C7—C4	123.86 (14)	C9—C14—H14	119.8
C7—N1—N2—C8	−163.47 (13)	N1—N2—C8—C9	−179.73 (12)
O1—C1—C2—C3	−177.79 (12)	N2—C8—C9—C10	−176.21 (15)
C6—C1—C2—C3	2.5 (2)	N2—C8—C9—C14	4.1 (2)
C1—C2—C3—C4	−0.7 (2)	C14—C9—C10—C11	−0.4 (2)
C2—C3—C4—C5	−1.6 (2)	C8—C9—C10—C11	179.94 (14)
C2—C3—C4—C7	179.70 (13)	C9—C10—C11—C12	0.8 (2)
C3—C4—C5—C6	2.2 (2)	C10—C11—C12—O2	−179.88 (14)
C7—C4—C5—C6	−179.07 (13)	C10—C11—C12—C13	−0.5 (2)
C4—C5—C6—C1	−0.4 (2)	O2—C12—C13—C14	179.33 (14)
O1—C1—C6—C5	178.33 (13)	C11—C12—C13—C14	0.0 (2)
C2—C1—C6—C5	−1.9 (2)	C12—C13—C14—C9	0.4 (2)
N2—N1—C7—C4	179.69 (12)	C10—C9—C14—C13	−0.2 (2)
C3—C4—C7—N1	−9.1 (2)	C8—C9—C14—C13	179.45 (14)

C5—C4—C7—N1	172.24 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···H2O^{i}	0.84 (10)	1.11 (10)	1.9303 (16)	163 (1)
O1—H1O···O2^{i}	0.84 (10)	1.94 (10)	2.7679 (16)	169 (1)
O2—H2O···H1O^{ii}	0.84 (10)	1.11 (10)	1.9393 (15)	168 (1)
O2—H2O···O1^{ii}	0.84 (10)	1.93 (10)	2.7679 (16)	175 (1)

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

Fig. 1

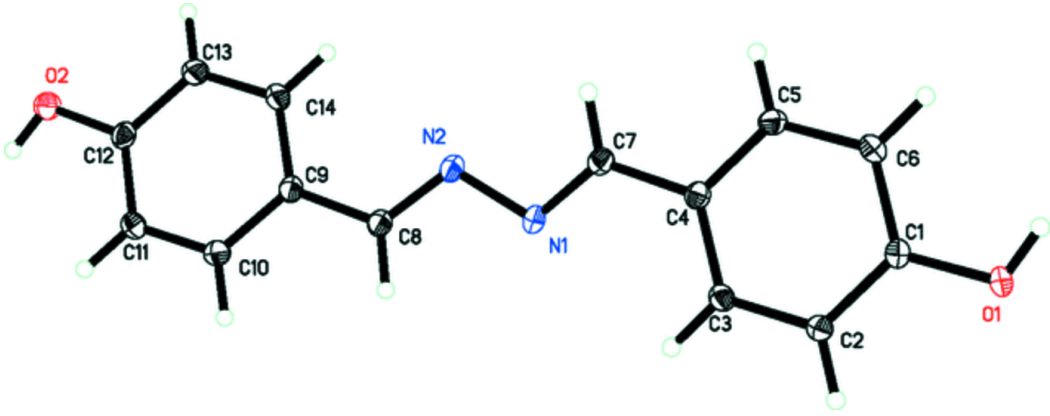

Fig. 2