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4-Hydroxy-3-nitrobenzaldehyde

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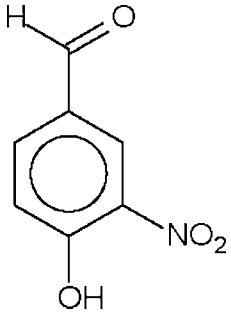
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.121; data-to-parameter ratio = 13.6.

The hydroxyl group in each of the two independent molecules of the title compound, $C_7H_5NO_4$, participates in two O—H···O hydrogen bonds, *viz.* one intramolecular bond to the nitro group and one intermolecular bond to the aldehyde group of the same molecule in the next unit, resulting in a linear chain structure. The dihedral angle between the aromatic ring and the nitro group is 10.9 (3)° in one molecule and 9.9 (2)° in the other.

Related literature

For the structure of 2-nitrophenol, see: Iwasaki & Kawano (1978). For the structure of 4-hydroxybenzaldehyde, see: Jasinski *et al.* (2008).



Experimental

Crystal data

$C_7H_5NO_4$
M_r = 167.12
Triclinic, $P\overline{1}$
a = 8.042 (1) Å
b = 8.036 (1) Å
c = 12.242 (2) Å
α = 71.975 (2)°
β = 70.820 (2)°
γ = 67.323 (2)°
V = 674.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 100 (2) K
0.40 × 0.05 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
4245 measured reflections
3068 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
S = 0.99
3068 reflections
225 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*o*···O1^{i}	0.84 (1)	2.13 (3)	2.676 (2)	122 (3)
O4—H4*o*···O3	0.84 (1)	1.91 (2)	2.638 (2)	144 (3)
O8—H8*o*···O5^{ii}	0.84 (1)	2.10 (3)	2.687 (2)	128 (3)
O8—H8*o*···O7	0.84 (1)	1.94 (2)	2.635 (2)	139 (3)

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

We thank the University of Malaya for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2191).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
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Iwasaki, F. & Kawano, Y. (1978). *Acta Cryst.* B**34**, 1286–1290.
Jasinski, J. P., Butcher, R. J., Narayana, B., Swamy, M. T. & Yathirajan, H. S. (2008). *Acta Cryst.* E**64**, o187.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o915 [doi:10.1107/S1600536808011148]

4-Hydroxy-3-nitrobenzaldehyde

Mohd. Razali Rizal, Isha Azizul and Seik Weng Ng

S1. Comment

A nitro group either *ortho* or *para* to a hydroxyl group can significantly increase the acidity of the resulting phenol. The crystal structures of a large number of 2-nitrophenol compounds have reported; the title compound represents another example. The hydroxyl group of the two independent molecules of the title compound (Fig. 1) is intramolecularly linked to the nitro group by an O–H···O hydrogen bond; the hydroxy group is intermolecularly linked to the aldehyde group of the molecule in the next unit cell by an similar hydrogen bond to result in a linear chain structure (Fig. 2). 2-Nitrophenol itself features an intramolecular hydrogen bond of 2.602 Å (Iwasaki & Kawano, 1978). On the other hand, 4-hydroxy-benzaldehyde exists as a hydrogen-bonded chain [O–H···O 2.731 (2) Å] (Jasinski *et al.*, 2008).

S2. Experimental

The commercially available compound (Sigma Aldrich) was recrystallized from water.

S3. 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 hydroxy H-atoms were located in a difference Fourier map, and were refined with an O–H distance restraint of 0.84±0.01 Å; their temperature factors were freely refined.

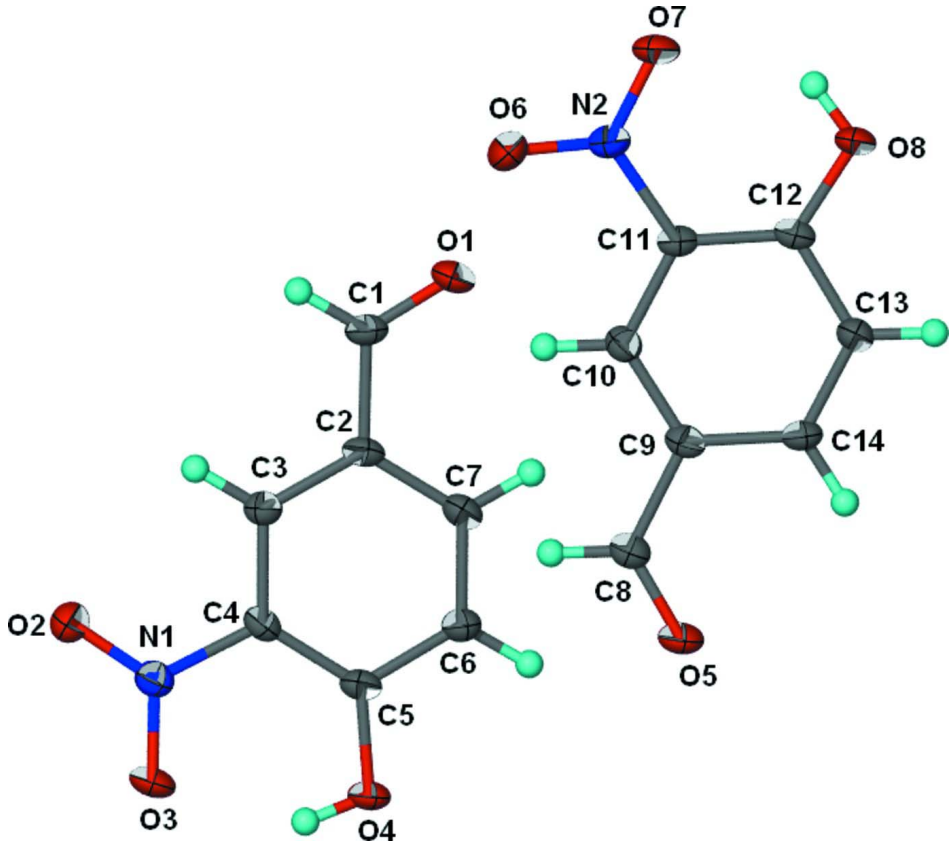

Figure 1

Thermal ellipsoid plot of the two independent molecules of the title compound at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

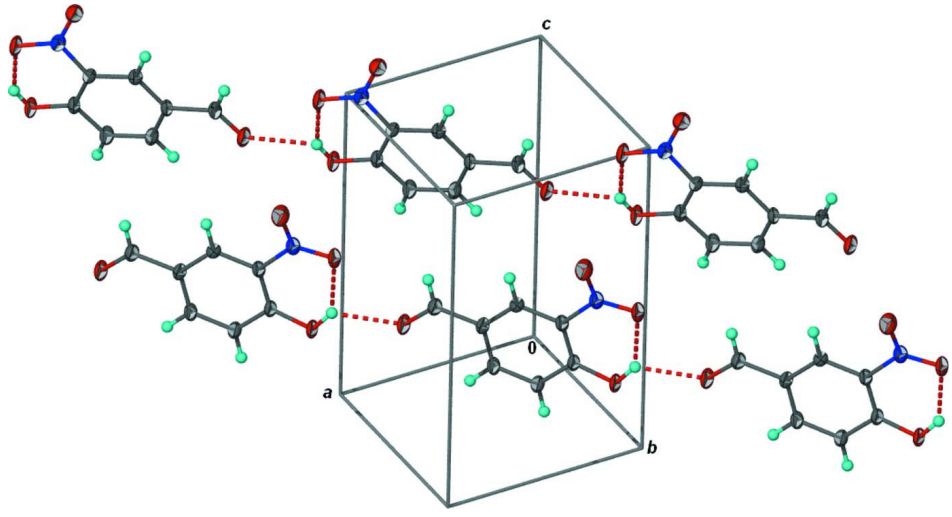

Figure 2

Chain structure of 4-hydroxy-3-nitrobenzaldehyde. Dashed lines denote hydrogen bonds.

4-Hydroxy-3-nitrobenzaldehyde

Crystal data

$C_7H_5NO_4$
$M_r = 167.12$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.042$ (1) Å
$b = 8.036$ (1) Å
$c = 12.242$ (2) Å
$\alpha = 71.975$ (2)°
$\beta = 70.820$ (2)°
$\gamma = 67.323$ (2)°
$V = 674.1$ (2) Å^3
$Z = 4$
$F(000) = 344$
$D_x = 1.647$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1123 reflections
$\theta = 3.0$–$28.8°$
$\mu = 0.14$ mm^{-1}
$T = 100$ K
Prism, yellow
0.40 × 0.05 × 0.05 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4245 measured reflections
3068 independent reflections
2134 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.121$
$S = 0.99$
3068 reflections
225 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.2315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4321 (2)	0.8384 (2)	0.8786 (1)	0.0221 (3)
O2	0.9772 (2)	0.2412 (2)	1.1704 (1)	0.0225 (4)
O3	1.1859 (2)	0.0816 (2)	1.0449 (1)	0.0224 (4)
O4	1.1227 (2)	0.1121 (2)	0.8402 (1)	0.0204 (3)
O5	1.0630 (2)	0.6755 (2)	0.4971 (1)	0.0220 (3)
O6	0.4719 (2)	1.2568 (2)	0.7806 (1)	0.0277 (4)
O7	0.2851 (2)	1.4257 (2)	0.6664 (1)	0.0231 (4)
O8	0.3813 (2)	1.4045 (2)	0.4424 (1)	0.0199 (3)
N1	1.0379 (2)	0.2049 (2)	1.0719 (2)	0.0173 (4)
N2	0.4272 (2)	1.2985 (2)	0.6866 (2)	0.0189 (4)
C1	0.5276 (3)	0.7418 (3)	0.9488 (2)	0.0175 (4)
C2	0.6821 (3)	0.5734 (3)	0.9247 (2)	0.0157 (4)

C3	0.7856 (3)	0.4675 (3)	1.0075 (2)	0.0160 (4)
C4	0.9342 (3)	0.3115 (3)	0.9816 (2)	0.0153 (4)
C5	0.9815 (3)	0.2577 (3)	0.8741 (2)	0.0162 (4)
C6	0.8705 (3)	0.3642 (3)	0.7931 (2)	0.0193 (4)
C7	0.7247 (3)	0.5181 (3)	0.8181 (2)	0.0185 (4)
C8	0.9568 (3)	0.7675 (3)	0.5691 (2)	0.0181 (4)
C9	0.8044 (3)	0.9364 (3)	0.5399 (2)	0.0157 (4)
C10	0.6886 (3)	1.0378 (3)	0.6244 (2)	0.0157 (4)
C11	0.5444 (3)	1.1966 (3)	0.5950 (2)	0.0157 (4)
C12	0.5144 (3)	1.2565 (3)	0.4804 (2)	0.0155 (4)
C13	0.6380 (3)	1.1535 (3)	0.3950 (2)	0.0174 (4)
C14	0.7784 (3)	0.9973 (3)	0.4242 (2)	0.0173 (4)
H4o	1.185 (4)	0.068 (4)	0.892 (2)	0.06 (1)*
H8o	0.308 (3)	1.452 (4)	0.499 (2)	0.05 (1)*
H1	0.5013	0.7765	1.0216	0.021*
H3	0.7557	0.5010	1.0812	0.019*
H6	0.8969	0.3290	0.7203	0.023*
H7	0.6514	0.5884	0.7623	0.022*
H8	0.9724	0.7290	0.6477	0.022*
H10	0.7070	0.9998	0.7023	0.019*
H13	0.6238	1.1931	0.3161	0.021*
H14	0.8593	0.9290	0.3655	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0187 (8)	0.0176 (8)	0.0236 (8)	0.0041 (6)	−0.0081 (6)	−0.0052 (6)
O2	0.0246 (8)	0.0218 (8)	0.0174 (7)	−0.0016 (7)	−0.0057 (6)	−0.0057 (6)
O3	0.0171 (8)	0.0177 (8)	0.0261 (8)	0.0048 (6)	−0.0082 (6)	−0.0059 (6)
O4	0.0169 (8)	0.0172 (8)	0.0234 (8)	0.0048 (6)	−0.0073 (6)	−0.0096 (6)
O5	0.0191 (8)	0.0171 (8)	0.0251 (8)	0.0038 (6)	−0.0071 (6)	−0.0083 (6)
O6	0.0294 (9)	0.0283 (9)	0.0199 (8)	0.0037 (7)	−0.0080 (7)	−0.0121 (7)
O7	0.0175 (8)	0.0186 (8)	0.0241 (8)	0.0047 (6)	−0.0035 (6)	−0.0075 (6)
O8	0.0155 (8)	0.0171 (7)	0.0197 (8)	0.0049 (6)	−0.0051 (6)	−0.0060 (6)
N1	0.0170 (9)	0.0152 (9)	0.0187 (9)	−0.0028 (7)	−0.0058 (7)	−0.0035 (7)
N2	0.0171 (9)	0.0166 (9)	0.0189 (9)	−0.0004 (7)	−0.0029 (7)	−0.0063 (7)
C1	0.0149 (10)	0.0145 (10)	0.0201 (10)	−0.0005 (8)	−0.0023 (8)	−0.0065 (8)
C2	0.0104 (9)	0.0135 (10)	0.0198 (10)	−0.0007 (8)	−0.0025 (8)	−0.0040 (8)
C3	0.0149 (10)	0.0149 (10)	0.0163 (10)	−0.0025 (8)	−0.0033 (8)	−0.0038 (8)
C4	0.0134 (10)	0.0138 (10)	0.0167 (10)	−0.0026 (8)	−0.0055 (8)	−0.0006 (8)
C5	0.0117 (10)	0.0142 (10)	0.0204 (10)	−0.0006 (8)	−0.0038 (8)	−0.0048 (8)
C6	0.0177 (11)	0.0187 (11)	0.0197 (10)	0.0010 (8)	−0.0060 (9)	−0.0085 (8)
C7	0.0149 (10)	0.0175 (10)	0.0202 (10)	−0.0001 (8)	−0.0070 (8)	−0.0034 (8)
C8	0.0167 (10)	0.0153 (10)	0.0199 (10)	−0.0018 (8)	−0.0057 (8)	−0.0034 (8)
C9	0.0145 (10)	0.0119 (10)	0.0195 (10)	−0.0020 (8)	−0.0054 (8)	−0.0031 (8)
C10	0.0154 (10)	0.0147 (10)	0.0155 (10)	−0.0034 (8)	−0.0047 (8)	−0.0017 (8)
C11	0.0132 (10)	0.0135 (10)	0.0182 (10)	−0.0018 (8)	−0.0021 (8)	−0.0053 (8)
C12	0.0123 (10)	0.0121 (9)	0.0196 (10)	−0.0013 (8)	−0.0040 (8)	−0.0032 (8)

C13	0.0153 (10)	0.0170 (10)	0.0171 (10)	0.0000 (8)	−0.0057 (8)	−0.0043 (8)
C14	0.0150 (10)	0.0152 (10)	0.0189 (10)	0.0006 (8)	−0.0033 (8)	−0.0075 (8)

Geometric parameters (Å, º)

O1—C1	1.222 (2)	C8—C9	1.475 (3)
O2—N1	1.223 (2)	C9—C10	1.380 (3)
O3—N1	1.242 (2)	C9—C14	1.406 (3)
O4—C5	1.341 (2)	C10—C11	1.397 (3)
O5—C8	1.214 (3)	C11—C12	1.405 (3)
O6—N2	1.226 (2)	C12—C13	1.408 (3)
O7—N2	1.241 (2)	C13—C14	1.368 (3)
O8—C12	1.335 (2)	O4—H4o	0.84 (1)
N1—C4	1.457 (3)	O8—H8o	0.84 (1)
N2—C11	1.447 (3)	C1—H1	0.9500
C1—C2	1.473 (3)	C3—H3	0.9500
C2—C3	1.385 (3)	C6—H6	0.9500
C2—C7	1.403 (3)	C7—H7	0.9500
C3—C4	1.394 (3)	C8—H8	0.9500
C4—C5	1.399 (3)	C10—H10	0.9500
C5—C6	1.408 (3)	C13—H13	0.9500
C6—C7	1.370 (3)	C14—H14	0.9500
O2—N1—O3	122.8 (2)	C10—C11—N2	117.7 (2)
O2—N1—C4	119.0 (2)	C12—C11—N2	121.0 (2)
O3—N1—C4	118.1 (2)	O8—C12—C11	126.7 (2)
O6—N2—O7	122.6 (2)	O8—C12—C13	115.7 (2)
O6—N2—C11	119.1 (2)	C11—C12—C13	117.7 (2)
O7—N2—C11	118.3 (2)	C14—C13—C12	120.9 (2)
O1—C1—C2	122.4 (2)	C13—C14—C9	120.9 (2)
C3—C2—C7	119.4 (2)	C5—O4—H4o	106 (2)
C3—C2—C1	120.4 (2)	C12—O8—H8o	110 (2)
C7—C2—C1	120.3 (2)	O1—C1—H1	118.8
C2—C3—C4	119.4 (2)	C2—C1—H1	118.8
C3—C4—C5	121.8 (2)	C2—C3—H3	120.3
C3—C4—N1	117.1 (2)	C4—C3—H3	120.3
C5—C4—N1	121.1 (2)	C7—C6—H6	119.7
O4—C5—C4	126.4 (2)	C5—C6—H6	119.7
O4—C5—C6	115.9 (2)	C6—C7—H7	119.5
C4—C5—C6	117.7 (2)	C2—C7—H7	119.5
C7—C6—C5	120.6 (2)	O5—C8—H8	118.5
C6—C7—C2	121.1 (2)	C9—C8—H8	118.5
O5—C8—C9	122.9 (2)	C9—C10—H10	120.1
C10—C9—C14	119.4 (2)	C11—C10—H10	120.1
C10—C9—C8	120.8 (2)	C14—C13—H13	119.5
C14—C9—C8	119.8 (2)	C12—C13—H13	119.5
C9—C10—C11	119.8 (2)	C13—C14—H14	119.6
C10—C11—C12	121.3 (2)	C9—C14—H14	119.6

O1—C1—C2—C3	−179.5 (2)	O5—C8—C9—C10	−179.1 (2)
O1—C1—C2—C7	0.0 (3)	O5—C8—C9—C14	−0.3 (3)
C7—C2—C3—C4	2.1 (3)	C14—C9—C10—C11	1.7 (3)
C1—C2—C3—C4	−178.3 (2)	C8—C9—C10—C11	−179.5 (2)
C2—C3—C4—C5	−0.4 (3)	C9—C10—C11—C12	−0.3 (3)
C2—C3—C4—N1	−179.8 (2)	C9—C10—C11—N2	−179.8 (2)
O2—N1—C4—C3	9.5 (3)	O6—N2—C11—C10	9.2 (3)
O3—N1—C4—C3	−169.8 (2)	O7—N2—C11—C10	−171.1 (2)
O2—N1—C4—C5	−170.0 (2)	O6—N2—C11—C12	−170.3 (2)
O3—N1—C4—C5	10.7 (3)	O7—N2—C11—C12	9.4 (3)
C3—C4—C5—O4	179.0 (2)	C10—C11—C12—O8	179.6 (2)
N1—C4—C5—O4	−1.6 (3)	N2—C11—C12—O8	−0.9 (3)
C3—C4—C5—C6	−1.6 (3)	C10—C11—C12—C13	−1.6 (3)
N1—C4—C5—C6	177.8 (2)	N2—C11—C12—C13	177.9 (2)
O4—C5—C6—C7	−178.7 (2)	O8—C12—C13—C14	−179.0 (2)
C4—C5—C6—C7	1.9 (3)	C11—C12—C13—C14	2.1 (3)
C5—C6—C7—C2	−0.1 (3)	C12—C13—C14—C9	−0.8 (3)
C3—C2—C7—C6	−2.0 (3)	C10—C9—C14—C13	−1.2 (3)
C1—C2—C7—C6	178.5 (2)	C8—C9—C14—C13	180.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*o*···O1^{i}	0.84 (1)	2.13 (3)	2.676 (2)	122 (3)
O4—H4*o*···O3	0.84 (1)	1.91 (2)	2.638 (2)	144 (3)
O8—H8*o*···O5^{ii}	0.84 (1)	2.10 (3)	2.687 (2)	128 (3)
O8—H8*o*···O7	0.84 (1)	1.94 (2)	2.635 (2)	139 (3)

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