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2,3,4-Trihydroxybenzaldehyde

Seik Weng Ng

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

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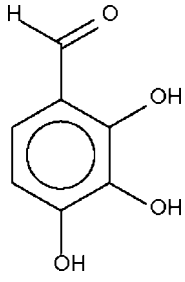
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.008 Å; R factor = 0.054; wR factor = 0.132; data-to-parameter ratio = 6.9.

The title compound, $C_7H_6O_4$, crystallizes with two independent molecules in the asymmetric unit. In both molecules, the 2-hydroxy group is bound *via* intramolecular hydrogen bonds to the aldehyde group. The molecules interact through O—H···O hydrogen bonds to form a three-dimensional network structure; each hydroxy group serves as a donor to only one acceptor atom.

Related literature

For some references on hydroxy-substituted benzaldehydes, see: Kretz *et al.* (2007); Ng (2005). For the crystal structures of Schiff base derivatives of 2,3,4-trihydroxysalicylaldehyde, see: Petek *et al.* (2006); Sun *et al.* (2007).



Experimental

Crystal data

$C_7H_6O_4$
M_r = 154.12
Monoclinic, Cc
a = 3.6222 (3) Å
b = 24.006 (2) Å
c = 14.8965 (9) Å
β = 93.524 (5)°
V = 1292.9 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 100 (2) K
0.30 × 0.03 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
5464 measured reflections
1491 independent reflections
1087 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.132
S = 1.01
1491 reflections
217 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 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
O2—H2···O1	0.84 (1)	1.99 (5)	2.631 (5)	133 (6)
O3—H3···O7^{i}	0.84 (1)	2.04 (3)	2.816 (5)	153 (6)
O4—H4···O1^{ii}	0.84 (1)	1.90 (3)	2.701 (5)	159 (6)
O6—H6···O5	0.84 (1)	1.87 (3)	2.653 (5)	154 (6)
O7—H7···O2	0.84 (1)	2.02 (3)	2.772 (5)	149 (6)
O8—H8···O5^{iii}	0.84 (1)	1.86 (2)	2.679 (5)	162 (7)

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

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).

I thank the University of Malaya for supporting this study through the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2748).

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supplementary materials

Acta Cryst. (2008). E**64**, o1565 [**doi:10.1107/S1600536808022241**]

2,3,4-Trihydroxybenzaldehyde

S. W. Ng

Comment

2,3,4-Trihydroxybenzaldehyde condenses with primary amines to afford Schiff bases. The crystal structures of only few such Schiff bases have been reported. The 2-fluoroaniline derivative exists as a zwitterion as the hydrogen atom of the 2-hydroxy substituent is transferred to the imino nitrogen atom (Petek *et al.*, 2006). On the other hand, the antipyrine derivative has the expected neutral structure (Sun *et al.*, 2007). Although there are several structural studies on hydroxy-substituted benzaldehydes (Kretz *et al.*, 2007; Ng, 2005), the structure of 2,3,4-trihydroxybenzaldehyde has not been reported.

2,3,4-Trihydroxybenzaldehyde (Scheme I) crystallizes with two independent molecules in the asymmetric unit. In both, the 2-hydroxy group is hydrogen-bonded to the aldehyde group via an intramolecular hydrogen bond (Fig. 1). The molecules interact through O–H···O hydrogen bonds to form a three-dimensional network structure; each hydroxy group serves as donor to only one acceptor atom.

Experimental

Commercially available 2,3,4-trihydroxybenzaldehyde was recrystallized from ethanol to furnished light-brown, needled-shaped crystals.

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_{eq}(C). The hydroxy H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their displacement parameters were set to 1.5U_{eq}(O).

Figures

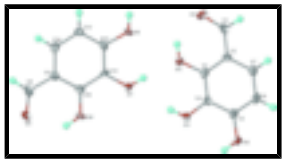

Fig. 1. Plot (Barbour, 2001) of the two independent molecules of 2,3,4-trihydroxybenzaldehyde with 50% probability ellipsoids. Hydrogen atoms are drawn as spheres of arbitrary radius.

2,3,4-Trihydroxybenzaldehyde

Crystal data

$C_7H_6O_4$	F_{000} = 640
M_r = 154.12	D_x = 1.584 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation

	λ = 0.71073 Å
Hall symbol: C c	Cell parameters from 446 reflections
a = 3.6222 (3) Å	θ = 2.8–19.5º
b = 24.006 (2) Å	μ = 0.13 mm^{-1}
c = 14.8965 (9) Å	T = 100 (2) K
β = 93.524 (5)º	Needle, light brown
V = 1292.9 (2) Å^3	0.30 × 0.03 × 0.03 mm
Z = 8	

Data collection

Bruker SMART APEX diffractometer	1087 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.088
Monochromator: graphite	θ_{max} = 27.5º
T = 100(2) K	θ_{min} = 1.7º
ω scans	h = −4→3
Absorption correction: None	k = −30→30
5464 measured reflections	l = −19→19
1491 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
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 2.3366P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
1491 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
217 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
8 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Friedel pairs were merged

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.5000 (11)	0.19999 (15)	0.5000 (3)	0.0203 (9)
O2	0.4561 (11)	0.18738 (14)	0.6744 (3)	0.0177 (9)
H2	0.432 (19)	0.172 (2)	0.6236 (19)	0.027*
O3	0.2999 (11)	0.23611 (14)	0.8356 (2)	0.0186 (9)
H3	0.253 (18)	0.2022 (8)	0.827 (4)	0.028*
O4	0.0704 (11)	0.34509 (15)	0.8358 (3)	0.0187 (9)
H4	0.046 (19)	0.324 (2)	0.879 (3)	0.028*
O5	1.4505 (11)	−0.00937 (16)	1.0289 (3)	0.0206 (9)

O6	1.1992 (11)	0.08512 (14)	0.9559 (2)	0.0195 (9)
H6	1.297 (17)	0.062 (2)	0.993 (3)	0.029*
O7	0.8968 (11)	0.13655 (14)	0.8094 (3)	0.0187 (9)
H7	0.801 (18)	0.142 (2)	0.7575 (19)	0.028*
O8	0.7396 (10)	0.07867 (14)	0.6555 (2)	0.0172 (9)
H8	0.696 (19)	0.056 (2)	0.613 (3)	0.026*
C1	0.3888 (16)	0.2489 (2)	0.5099 (4)	0.0182 (12)
H1	0.3571	0.2717	0.4579	0.022*
C2	0.3068 (15)	0.2725 (2)	0.5942 (4)	0.0140 (11)
C3	0.3431 (15)	0.2416 (2)	0.6752 (4)	0.0148 (11)
C4	0.2636 (16)	0.2646 (2)	0.7557 (4)	0.0151 (12)
C5	0.1496 (15)	0.3204 (2)	0.7578 (4)	0.0153 (11)
C6	0.1124 (15)	0.3520 (2)	0.6789 (4)	0.0171 (12)
H6A	0.0328	0.3896	0.6812	0.021*
C7	0.1914 (16)	0.3285 (2)	0.5982 (4)	0.0184 (12)
H7A	0.1680	0.3501	0.5448	0.022*
C8	1.3595 (16)	−0.0319 (2)	0.9554 (4)	0.0182 (12)
H8A	1.4039	−0.0707	0.9498	0.022*
C9	1.1938 (15)	−0.0035 (2)	0.8791 (4)	0.0146 (11)
C10	1.1232 (16)	0.0546 (2)	0.8814 (4)	0.0150 (11)
C11	0.9686 (16)	0.08085 (19)	0.8055 (4)	0.0142 (11)
C12	0.8902 (15)	0.0499 (2)	0.7274 (3)	0.0142 (11)
C13	0.9584 (15)	−0.0072 (2)	0.7239 (4)	0.0160 (12)
H13	0.9043	−0.0276	0.6701	0.019*
C14	1.1054 (15)	−0.0333 (2)	0.7999 (4)	0.0167 (12)
H14	1.1480	−0.0723	0.7988	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.023 (2)	0.0189 (19)	0.019 (2)	0.0023 (16)	0.0050 (18)	−0.0053 (15)
O2	0.025 (2)	0.0122 (17)	0.015 (2)	0.0033 (16)	−0.0038 (18)	−0.0012 (15)
O3	0.032 (3)	0.0111 (17)	0.013 (2)	0.0021 (16)	0.0006 (18)	0.0028 (14)
O4	0.027 (2)	0.0147 (17)	0.015 (2)	0.0041 (17)	0.0023 (17)	−0.0010 (15)
O5	0.023 (2)	0.023 (2)	0.015 (2)	0.0024 (17)	−0.0034 (17)	0.0012 (16)
O6	0.032 (3)	0.0147 (18)	0.011 (2)	−0.0003 (16)	−0.0070 (18)	−0.0039 (15)
O7	0.029 (3)	0.0124 (16)	0.0140 (18)	0.0040 (16)	−0.0032 (17)	−0.0030 (15)
O8	0.023 (2)	0.0163 (18)	0.011 (2)	0.0023 (16)	−0.0065 (17)	−0.0020 (14)
C1	0.017 (3)	0.020 (3)	0.017 (3)	0.001 (2)	−0.005 (3)	0.003 (2)
C2	0.010 (3)	0.018 (2)	0.014 (3)	0.001 (2)	0.000 (2)	−0.003 (2)
C3	0.007 (3)	0.015 (2)	0.022 (3)	0.002 (2)	−0.002 (2)	−0.002 (2)
C4	0.016 (3)	0.014 (2)	0.015 (3)	0.001 (2)	−0.002 (2)	0.001 (2)
C5	0.011 (3)	0.017 (3)	0.019 (3)	−0.001 (2)	0.003 (2)	−0.001 (2)
C6	0.014 (3)	0.012 (2)	0.025 (3)	0.002 (2)	0.000 (3)	0.000 (2)
C7	0.021 (3)	0.017 (3)	0.017 (3)	0.002 (2)	−0.001 (3)	0.003 (2)
C8	0.014 (3)	0.019 (3)	0.022 (3)	0.000 (2)	0.002 (2)	0.006 (2)
C9	0.012 (3)	0.015 (2)	0.016 (3)	0.000 (2)	0.001 (2)	0.001 (2)
C10	0.011 (3)	0.021 (3)	0.014 (3)	−0.002 (2)	0.000 (2)	−0.004 (2)

C11	0.013 (3)	0.012 (2)	0.017 (3)	0.000 (2)	0.001 (2)	−0.005 (2)
C12	0.009 (3)	0.020 (2)	0.014 (3)	0.000 (2)	0.000 (2)	0.003 (2)
C13	0.013 (3)	0.020 (3)	0.014 (3)	0.000 (2)	−0.002 (2)	−0.004 (2)
C14	0.012 (3)	0.014 (3)	0.024 (3)	0.001 (2)	−0.001 (2)	0.000 (2)

Geometric parameters (Å, °)

O1—C1	1.253 (6)	C9—C10	1.421 (7)
O2—C3	1.365 (6)	C10—C11	1.382 (8)
O3—C4	1.372 (6)	C11—C12	1.395 (7)
O4—C5	1.351 (6)	C12—C13	1.394 (7)
O5—C8	1.248 (7)	C13—C14	1.372 (7)
O6—C10	1.343 (6)	O2—H2	0.84 (1)
O7—C11	1.364 (6)	O3—H3	0.84 (1)
O8—C12	1.361 (6)	O4—H4	0.84 (1)
C1—C2	1.426 (7)	O6—H6	0.84 (1)
C2—C7	1.409 (7)	O7—H7	0.84 (1)
C2—C3	1.416 (7)	O8—H8	0.84 (1)
C3—C4	1.367 (7)	C1—H1	0.9500
C4—C5	1.402 (7)	C6—H6A	0.9500
C5—C6	1.398 (7)	C7—H7A	0.9500
C6—C7	1.374 (7)	C8—H8A	0.9500
C8—C9	1.425 (8)	C13—H13	0.9500
C9—C14	1.398 (7)	C14—H14	0.9500
C3—O2—H2	114 (4)	C10—C9—C8	121.1 (5)
C4—O3—H3	110 (5)	O6—C10—C11	118.6 (4)
C5—O4—H4	116 (5)	O6—C10—C9	121.9 (5)
C10—O6—H6	104 (4)	C11—C10—C9	119.5 (5)
C11—O7—H7	101 (4)	O7—C11—C10	118.7 (5)
C12—O8—H8	108 (4)	O7—C11—C12	121.9 (5)
O1—C1—C2	124.2 (5)	C10—C11—C12	119.4 (4)
C7—C2—C3	118.4 (5)	O8—C12—C13	122.3 (5)
C7—C2—C1	119.7 (5)	O8—C12—C11	115.9 (4)
C3—C2—C1	121.9 (4)	C13—C12—C11	121.9 (5)
O2—C3—C4	118.2 (5)	C14—C13—C12	118.6 (5)
O2—C3—C2	120.4 (5)	C13—C14—C9	121.3 (5)
C4—C3—C2	121.5 (4)	O1—C1—H1	117.9
C3—C4—O3	123.1 (4)	C2—C1—H1	117.9
C3—C4—C5	118.9 (5)	C7—C6—H6A	120.1
O3—C4—C5	118.0 (5)	C5—C6—H6A	120.1
O4—C5—C6	118.0 (5)	C6—C7—H7A	119.8
O4—C5—C4	121.1 (5)	C2—C7—H7A	119.8
C6—C5—C4	120.9 (5)	O5—C8—H8A	117.6
C7—C6—C5	119.9 (5)	C9—C8—H8A	117.6
C6—C7—C2	120.4 (5)	C14—C13—H13	120.7
O5—C8—C9	124.7 (5)	C12—C13—H13	120.7
C14—C9—C10	119.4 (5)	C13—C14—H14	119.3
C14—C9—C8	119.5 (5)	C9—C14—H14	119.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.84 (1)	1.99 (5)	2.631 (5)	133 (6)
O3—H3···O7^{i}	0.84 (1)	2.04 (3)	2.816 (5)	153 (6)
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O8—H8···O5^{iii}	0.84 (1)	1.86 (2)	2.679 (5)	162 (7)

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

Fig. 1