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2,5-Dihydroxybenzaldehyde

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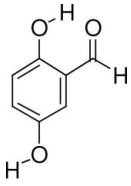
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 8.5.

The title compound, $C_7H_6O_3$, features a planar molecule (r.m.s. deviation for all non-H atoms = 0.019 Å). Geometric parameters are in the usual ranges. Whereas one hydroxyl group forms an intramolecular hydrogen bond with the carbonyl group, the other forms an intermolecular hydrogen bond with the carbonyl group of a symmetry-equivalent molecule. The molecules crystallize in planes parallel to the *bc* plane.

Related literature

For related literature, see: Kretz *et al.* (2006, 2007); Lerner *et al.* (2006); Margraf *et al.* (2006).



Experimental

Crystal data

$C_7H_6O_3$
M_r = 138.12
Orthorhombic, $P2_12_12_1$
a = 6.7544 (7) Å
b = 8.2240 (9) Å
c = 11.4040 (13) Å
V = 633.47 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 173 (2) K
0.49 × 0.32 × 0.29 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: none
7904 measured reflections
843 independent reflections
797 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.11
843 reflections
99 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O21^{i}	0.95 (3)	1.82 (3)	2.7382 (15)	163 (2)
O1—H1···O21	0.98 (2)	1.73 (3)	2.6501 (16)	155 (2)

Symmetry code: (i) $x, y-1, z$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2016).

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supplementary materials

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2,5-Dihydroxybenzaldehyde

T. Kretz, H.-W. Lerner and M. Bolte

Comment

Recently, we have extended our studies to redox-active ligands which can be used to influence the electrochemical reactivity of transition metals since their redox activity is expanded upon complexation (Lerner *et al.*, 2006; Kretz *et al.*, 2007). The resulting complexes can undergo multi-electron transfer reactions which are the sum of the oxidation state changes of the metal center and the ligand (Margraf *et al.*, 2006; Kretz *et al.*, 2006). Due to their electrochemical reversibility, hydroquinone / quinone derivatives are candidates for redox-active ligands (Lerner *et al.*, 2006; Kretz *et al.*, 2007). In our studies we have used Schiff-Base derivatives which can conveniently be achieved by reaction of amines and aldehyde derivatives (Margraf *et al.*, 2006; Kretz *et al.*, 2007). Thereby 2,5-dihydroxybenzaldehyde represents one of the starting materials. Single crystals of 2,5-dihydroxybenzaldehyde were obtained by recrystallization from toluene.

The title compound, $C_7H_6O_3$, features a planar molecule (r.m.s. deviation for all non-H atoms 0.019 Å). Geometric parameters are in the usual ranges. Whereas one hydroxyl group forms an intramolecular hydrogen bond with the carbonyl group, the other one forms an intermolecular hydrogen bond with the carbonyl group of a symmetry equivalent molecule. The molecules crystallize in planes parallel to the *bc* plane.

Experimental

Commercially available 2,5-dihydroxybenzaldehyde (1.38 g) was recrystallized from toluene (20 ml).

Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.93 Å. The H atoms bonded to O were refined isotropically. In the final cycles of refinement, in the absence of significant anomalous scattering effects, Friedel pairs were merged and Δf'' set to zero.

Figures

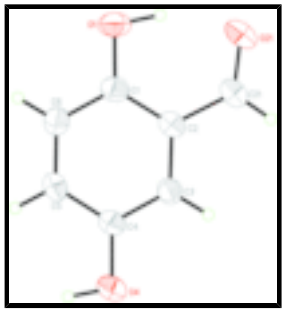

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

2,5-Dihydroxybenzaldehyde

Crystal data

$C_7H_6O_3$	F_{000} = 288
M_r = 138.12	D_x = 1.448 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 11598 reflections
a = 6.7544 (7) Å	θ = 3.8–27.4º
b = 8.2240 (9) Å	μ = 0.12 mm^{-1}
c = 11.4040 (13) Å	T = 173 (2) K
V = 633.47 (12) Å^3	Block, yellow
Z = 4	0.49 × 0.32 × 0.29 mm

Data collection

Stoe IPDS II two-circle diffractometer	797 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.064
Monochromator: graphite	θ_{max} = 27.3º
T = 173(2) K	θ_{min} = 3.9º
ω scans	h = −8→8
Absorption correction: none	k = −10→10
7904 measured reflections	l = −14→14
843 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.0216P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.084	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
843 reflections	Extinction correction: none
99 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Experimental. ;

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

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}
C1	0.1189 (2)	0.78697 (16)	0.40573 (13)	0.0313 (3)
C2	0.11078 (18)	0.80898 (15)	0.52767 (12)	0.0291 (3)
C3	0.1003 (2)	0.67401 (16)	0.60198 (12)	0.0303 (3)
H3	0.0964	0.6895	0.6845	0.036*
C4	0.0956 (2)	0.51869 (15)	0.55672 (12)	0.0306 (3)
C5	0.1033 (2)	0.49826 (15)	0.43446 (12)	0.0324 (3)
H5	0.0997	0.3916	0.4025	0.039*
C6	0.1159 (2)	0.62973 (16)	0.36011 (12)	0.0335 (3)
H6	0.1225	0.6133	0.2777	0.040*
O1	0.13038 (18)	0.91338 (14)	0.32977 (10)	0.0418 (3)
H1	0.119 (3)	1.005 (3)	0.384 (2)	0.064 (7)*
O4	0.0787 (2)	0.39039 (12)	0.63213 (10)	0.0435 (3)
H4	0.097 (4)	0.301 (3)	0.581 (2)	0.070 (7)*
C21	0.1097 (2)	0.97036 (17)	0.57875 (14)	0.0350 (3)
H21	0.1055	0.9793	0.6618	0.042*
O21	0.11390 (18)	1.09707 (11)	0.52045 (11)	0.0424 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0284 (6)	0.0292 (6)	0.0363 (7)	−0.0003 (6)	−0.0025 (5)	0.0039 (5)
C2	0.0263 (5)	0.0247 (6)	0.0363 (7)	0.0001 (6)	−0.0010 (5)	−0.0004 (5)
C3	0.0330 (6)	0.0271 (6)	0.0307 (6)	0.0008 (5)	−0.0015 (5)	−0.0021 (5)
C4	0.0320 (6)	0.0243 (6)	0.0356 (6)	0.0006 (5)	−0.0012 (5)	0.0025 (5)
C5	0.0341 (6)	0.0262 (6)	0.0371 (6)	0.0005 (5)	−0.0014 (5)	−0.0061 (5)
C6	0.0346 (6)	0.0351 (7)	0.0306 (6)	−0.0011 (6)	0.0001 (6)	−0.0032 (5)
O1	0.0508 (6)	0.0349 (5)	0.0396 (5)	−0.0017 (5)	−0.0021 (5)	0.0118 (4)
O4	0.0649 (8)	0.0240 (5)	0.0416 (5)	0.0002 (5)	−0.0014 (5)	0.0041 (4)
C21	0.0347 (6)	0.0252 (6)	0.0449 (7)	0.0011 (6)	0.0012 (6)	−0.0036 (5)
O21	0.0462 (5)	0.0231 (5)	0.0580 (7)	0.0010 (4)	0.0009 (5)	0.0017 (5)

Geometric parameters (Å, °)

C1—O1	1.3554 (16)	C4—C5	1.405 (2)
C1—C6	1.3941 (17)	C5—C6	1.3766 (19)

C1—C2	1.4034 (18)	C5—H5	0.9500
C2—C3	1.3982 (19)	C6—H6	0.9500
C2—C21	1.4494 (17)	O1—H1	0.98 (2)
C3—C4	1.3781 (17)	O4—H4	0.95 (3)
C3—H3	0.9500	C21—O21	1.2364 (18)
C4—O4	1.3660 (16)	C21—H21	0.9500
O1—C1—C6	118.28 (12)	C6—C5—C4	121.30 (11)
O1—C1—C2	122.45 (12)	C6—C5—H5	119.4
C6—C1—C2	119.27 (12)	C4—C5—H5	119.4
C3—C2—C1	120.01 (12)	C5—C6—C1	119.97 (12)
C3—C2—C21	118.89 (12)	C5—C6—H6	120.0
C1—C2—C21	121.10 (12)	C1—C6—H6	120.0
C4—C3—C2	120.66 (12)	C1—O1—H1	100.7 (14)
C4—C3—H3	119.7	C4—O4—H4	101.5 (16)
C2—C3—H3	119.7	O21—C21—C2	123.75 (13)
O4—C4—C3	118.82 (12)	O21—C21—H21	118.1
O4—C4—C5	122.37 (12)	C2—C21—H21	118.1
C3—C4—C5	118.79 (12)		
O1—C1—C2—C3	−179.61 (11)	O4—C4—C5—C6	178.53 (12)
C6—C1—C2—C3	0.2 (2)	C3—C4—C5—C6	0.2 (2)
O1—C1—C2—C21	1.4 (2)	C4—C5—C6—C1	−0.7 (2)
C6—C1—C2—C21	−178.79 (12)	O1—C1—C6—C5	−179.65 (12)
C1—C2—C3—C4	−0.8 (2)	C2—C1—C6—C5	0.5 (2)
C21—C2—C3—C4	178.24 (13)	C3—C2—C21—O21	−178.30 (13)
C2—C3—C4—O4	−177.85 (12)	C1—C2—C21—O21	0.7 (2)
C2—C3—C4—C5	0.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O21^{i}	0.95 (3)	1.82 (3)	2.7382 (15)	163 (2)
O1—H1···O21	0.98 (2)	1.73 (3)	2.6501 (16)	155 (2)

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1