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2,3-Dihydroxybenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.111
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Hydrogen bonds link planar molecules of 2,3-dihydroxybenzaldehyde, $C_7H_6O_3$, into ribbons.

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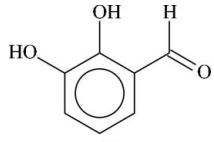
Comment

This study on 2,3-dihydroxybenzaldehyde, (I), follows those on 2,4-dihydroxybenzaldehyde (Hu *et al.*, 1999) and 3,4-dihydroxybenzaldehyde (Sarma *et al.*, 2000). The reagent, like other substituted salicylaldehydes, when condensed with primary amines, furnishes salen-type bases that can be used for the preparation of metal complexes (Achard *et al.*, 2004; Verquin *et al.*, 2004). The compound exists as a planar molecule (Fig. 1). Hydrogen bonds (Table 1) link adjacent molecules into a ribbon (Fig. 2).



(I)

Experimental

The title compound was obtained commercially and was recrystallized from pyridine.

Crystal data

$C_7H_6O_3$
M_r = 138.12
Monoclinic, $P2_1/n$
a = 12.409 (3) Å
b = 3.768 (2) Å
c = 13.349 (3) Å
β = 104.42 (3)°
V = 604.5 (4) Å^3
Z = 4
D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4742 reflections
θ = 3.2–27.5°
μ = 0.12 mm^{-1}
T = 295 (2) K
Block, colorless
0.32 × 0.24 × 0.17 mm

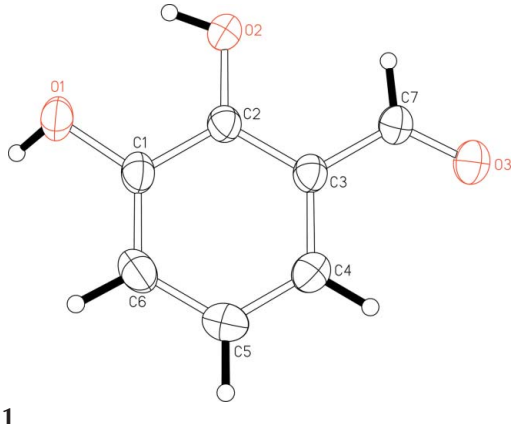


Figure 1
ORTEPII plot (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 50% probability level.

Data collection

Rigaki R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.794, T_{max} = 0.980
5427 measured reflections
1372 independent reflections
1193 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -4 \rightarrow 4$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.111
S = 1.09
1372 reflections
115 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.0682P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*o*···O3^{i}	0.86 (1)	1.80 (1)	2.648 (1)	174 (2)
O2—H2*o*···O1^{ii}	0.84 (1)	2.05 (1)	2.782 (1)	145 (2)

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.85 (1) Å and C—H = 0.95 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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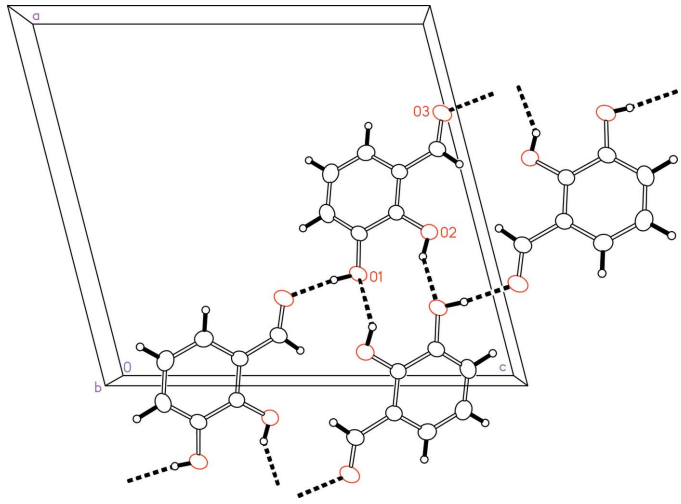

Figure 2
ORTEPII plot (Johnson, 1976) of the ribbon structure in (I). Dashed lines indicate hydrogen bonds.

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