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3,4-Methylenedioxybenzaldehyde

Shui Wang,[a]* Jing-Kang Wang[a] and Dong-Xiu Chen[b]

[a]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China, and [b]YiBin JianZhong Perfume Co. Ltd, Yibi 644000, People's Republic of China

Correspondence e-mail: lantianxia2000@sohu.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.119
Data-to-parameter ratio = 11.5

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

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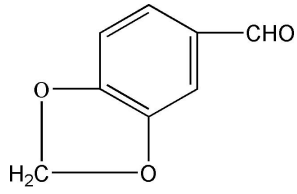
The title compound, $C_8H_6O_3$, is an important perfume and is also used as an important intermediate in the fine-chemical industry. All non-H atoms of the molecule are coplanar. In the crystal structure, the molecules are stacked parallel to the crystallographic (010) plane.

Comment

The title compound, (I), is an important perfume (Bi, 1989) and can be used as an important intermediate in the fine-chemical industry (Ohtaka *et al.*, 1988; Babudri *et al.*, 1991). Since its discovery in the 19th century, most studies have focused on its synthesis and application. To our knowledge, the single-crystal structure has not been reported before now. We present the crystal structure of (I) here.



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule consists of one six-membered ring and a fused five-membered ring. All non-H atoms of the molecule are coplanar.

In the crystal structure, the molecules are stacked parallel to the (010) plane (Fig. 2). No inter- or intramolecular hydrogen bonds are observed.

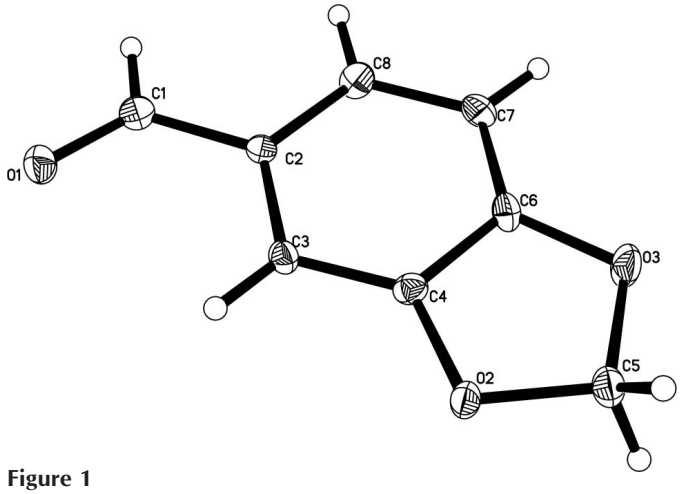


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

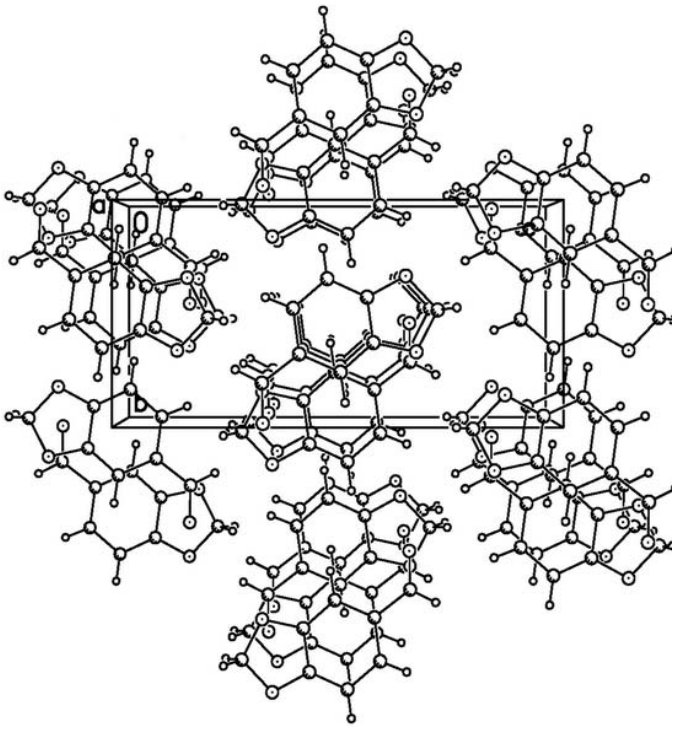


Figure 2
The molecular packing of (I), viewed along the *b* axis.

Experimental

3,4-Methylenedioxybenzaldehyde was provided by Yibin Jianzhong Chemicals Corporation, China. Its purity, as determined by gas chromatography, was better than 99.5%. The melting point, as determined by differential scanning calorimetry, was 310 K. Colourless plate-like single crystals of (I) suitable for X-ray diffraction were obtained by slow natural evaporation of an ethanol solution (10 ml) at room temperature.

Crystal data

$C_8H_6O_3$
M_r = 150.13
Orthorhombic, *Pnma*
a = 7.1738 (14) Å
b = 6.3367 (13) Å
c = 14.782 (3) Å
V = 672.0 (2) Å^3
Z = 4
D_x = 1.484 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6193 reflections
θ = 3.2–27.5°
μ = 0.12 mm^{-1}
T = 293 (2) K
Plate, colourless
0.79 × 0.19 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer
Oscillation scans
Absorption correction: ψ scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.914, T_{max} = 0.993
6628 measured reflections
840 independent reflections
631 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.5°
$h = -8 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 0.99
840 reflections
73 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.005 (3)

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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