

1,4-Benzenedimethanol

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Key indicators

Single-crystal X-ray study

 $T = 180\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$ R factor = 0.040 wR factor = 0.101

Data-to-parameter ratio = 12.5

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

The title compound, *p*-phenylenedimethanol, $\text{C}_8\text{H}_{10}\text{O}_2$, crystallizes in the space group $P2_1/n$ and forms extensive supramolecular sheets parallel to (001) via $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. Sheets stack along the *c* axis via weak $\text{C}-\text{H}\cdots\text{O}$ interactions. The molecule has no crystallographic symmetry.

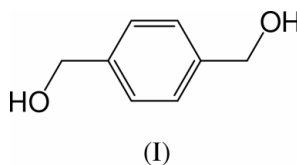
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Comment

1,4-Benzenedimethanol, (I), with molecular $\bar{1}$ (C_i) symmetry, is of interest in our study of crystal engineering because of the possible hydrogen-bonded packing arrangements it might adopt. Although numerous studies have been reported on the crystal structures of hydroquinone, with three polymorphs having been determined [the α -form (Lindeman *et al.*, 1981), the β -form (Wallwork & Powell, 1980) and the γ -form (Maartmann-Moe, 1966)], the structure of 1,4-benzenedimethanol has not yet been reported. We present here its crystal structure and show that the hydrogen-bond arrangement is similar to that of hydroquinone in its γ form.



The asymmetric unit of (I) consists of only one molecule (Fig. 1), with no crystallographic symmetry. In the crystal structure, the hydroxy groups are linked by $\text{O1}-\text{H01}\cdots\text{O2}^j$ and $\text{O2}-\text{H02}\cdots\text{O1}^{ii}$ hydrogen bonds alternately along the *a* axis (symmetry codes as in Table 1). Infinite supramolecular sheets are formed parallel to (001) (Fig. 2). Molecules of (I) pack in a herring-bone arrangement with the benzene rings seen edge-on along the *c* axis. The supramolecular sheets may then be considered to stack in an *ABAB* arrangement along the *c* axis, with $\text{C2}-\text{H2}\cdots\text{O1}^{iii}$ hydrogen bonds (symmetry code as in Table 1) linking the adjacent layers (Fig. 3).

Experimental

1,4-Benzenedimethanol was obtained from Aldrich. 20 mg of the complex was dissolved in 20 ml of ethanol. Crystals were obtained by slow evaporation of the solution at room temperature.

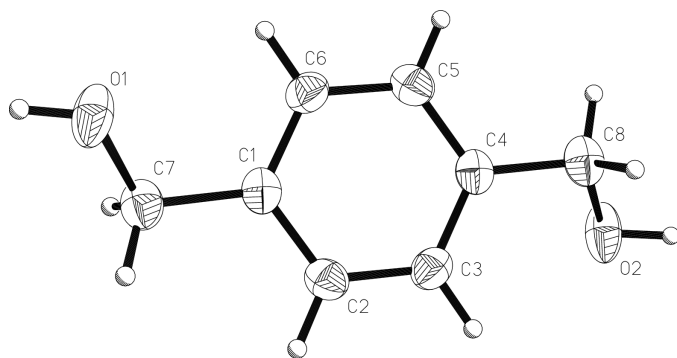


Figure 1
The molecular unit of (I) showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

Crystal data

$C_8H_{10}O_2$	$D_x = 1.289 \text{ Mg m}^{-3}$
$M_r = 138.16$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2696 reflections
$a = 4.8118(3) \text{ \AA}$	$\theta = 1.0\text{--}25.0^\circ$
$b = 15.4697(14) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 9.7712(8) \text{ \AA}$	$T = 180(2) \text{ K}$
$\beta = 101.798(5)^\circ$	Needle, colourless
$V = 711.97(10) \text{ \AA}^3$	$0.46 \times 0.10 \times 0.05 \text{ mm}$
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	974 reflections with $I > 2\sigma(I)$
Thin-slice ω and φ scans	$R_{\text{int}} = 0.043$
Absorption correction: multi-scan (<i>SORTAV</i> ; Blessing, 1995)	$\theta_{\text{max}} = 25.0^\circ$
$T_{\text{min}} = 0.890$, $T_{\text{max}} = 0.918$	$h = -5 \rightarrow 5$
4055 measured reflections	$k = -18 \rightarrow 18$
1238 independent reflections	$l = -9 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.1336P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.101$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
1238 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
99 parameters	
H atoms treated by a mixture of independent and constrained refinement	

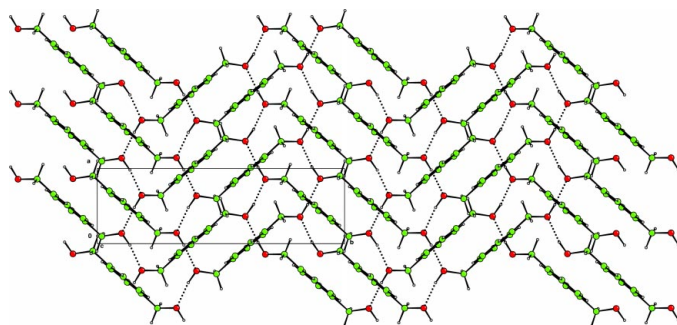


Figure 2
Projection on to (001) showing the supramolecular sheets formed by O—H...O hydrogen bonds of the hydroxy groups of (I) (*CAMERON*; Watkin *et al.*, 1996).

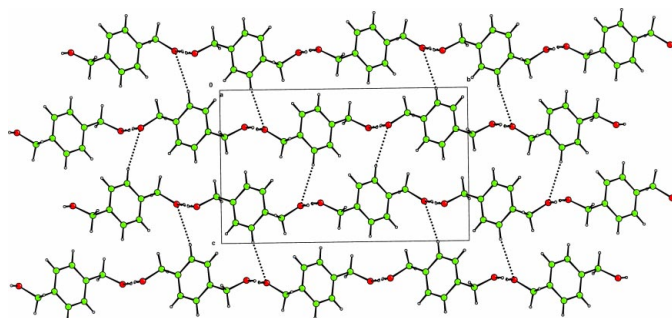


Figure 3
Projection on to (100) showing the stacking of the supramolecular sheets in an ABAB arrangement (*CAMERON*; Watkin *et al.*, 1996).

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1—H01...O2 ⁱ	0.90 (3)	1.82 (3)	2.7138 (15)	174 (2)
O2—H02...O1 ⁱⁱ	0.92 (2)	1.81 (3)	2.7238 (14)	170 (2)
C2—H2...O1 ⁱⁱⁱ	0.95	2.70	3.566 (2)	152

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

All H atoms bonded to C atoms were positioned geometrically and refined using a riding model with the U_{iso} values for each H atom taken as 1.2 U_{eq} of the carrier atom. H01 and H02, bonded to oxygen, were located from a difference Fourier map and refined freely.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL97*.

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