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Hexakis(hydroxymethyl)benzene

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The centrosymmetric title compound, $C_{12}H_{18}O_6$, exhibits a three-dimensional network structure. The structure displays extensive O—H···O hydrogen bonding. In each molecule, two sets of three neighboring hydroxy groups are located above and below the plane defined by the central benzene ring.

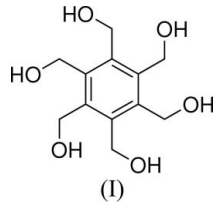
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.166
Data-to-parameter ratio = 13.4

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

Comment

The title compound, (I) (Fig. 1), forms a hydrogen-bonded three-dimensional network in the solid state (Table 1). Figs. 2 and 3 illustrate the packing viewed along the *a* and *b* axes.



(I)

Experimental

The title compound was prepared according to a published procedure and recrystallized from methanol (Alphonse *et al.*, 1988).

Crystal data

$C_{12}H_{18}O_6$
M_r = 258.26
Monoclinic, $P2_1/c$
a = 4.5946 (9) Å
b = 8.9294 (18) Å
c = 13.452 (3) Å
β = 95.50 (3)°
V = 549.35 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 120 (2) K
0.50 × 0.30 × 0.10 mm

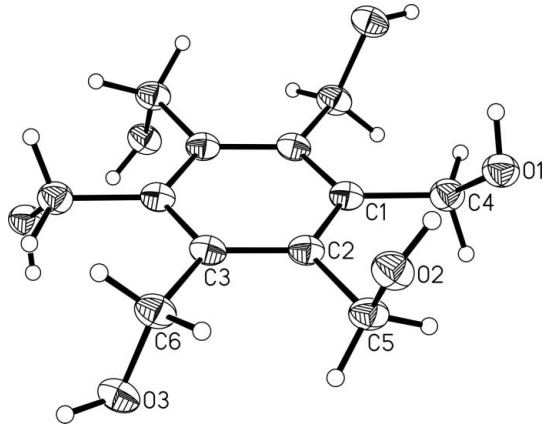


Figure 1
The molecular structure of (I) (displacement ellipsoids are at the 50% probability level). H atoms are drawn as spheres of arbitrary radius.

Data collection

Stoe IPDSII diffractometer
Absorption correction: none
4212 measured reflections
1143 independent reflections
868 reflections with $I > 2\sigma(I)$
$R_{int} = 0.088$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.166$
$S = 0.96$
1143 reflections
85 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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	2.34	2.951 (2)	130
O1—H1···O2^{i}	0.84	1.92	2.739 (2)	165
O1—H1···O3^{ii}	0.84	2.71	3.049 (3)	106
O2—H2···O3^{ii}	0.84	2.18	2.906 (3)	145
O3—H3···O1^{iii}	0.84	1.95	2.767 (2)	163

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

H atoms were treated as riding, with C—H = 0.99 Å, O—H = 0.84 Å and U_{iso}(H) values set at $1.2U_{eq}$(C) and $1.5U_{eq}$(O).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Alphonse, P., Moyen, F. & Mazerolles, P. (1988). *J. Organomet. Chem.* **345**, 209–216.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

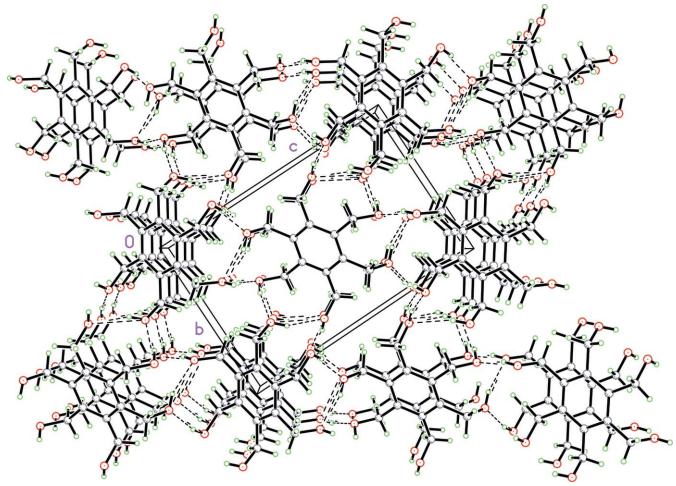

Figure 2
Packing diagram of (I) (viewed along the *a* axis). Hydrogen bonding is indicated by dashed lines.

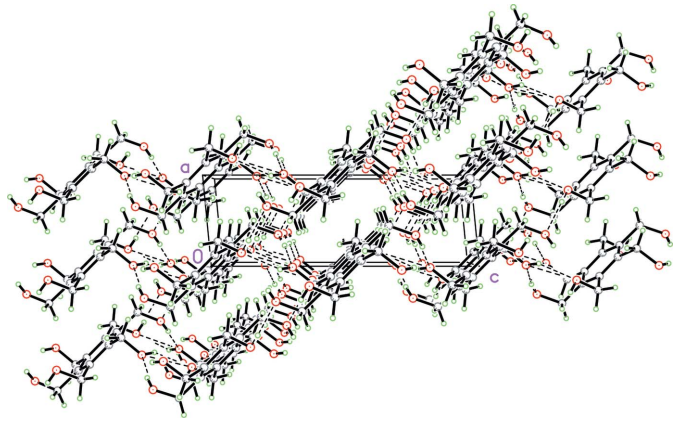

Figure 3
Packing diagram of 1 (viewed along the *b* axis). Hydrogen bonding is indicated by dashed lines.

Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.