

1,4-Bis(benzyloxy)benzene

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Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å

R factor = 0.042

wR factor = 0.138

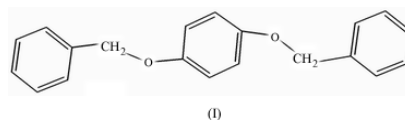
Data-to-parameter ratio = 12.3

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

The structure of the title compound, $\text{C}_{20}\text{H}_{18}\text{O}_2$, has been determined previously [Zaslow & Dubchansky (1967). *Mol. Cryst.* **3**, 297–298], but no three-dimensional coordinates are available. The molecule contains a crystallographic inversion center which lies in the middle of the central benzene ring.

Comment

Crystals of the title compound, (I), were isolated from the marine algae *Hydroclathrus Tenuis* collected from the Xisha Islands in the South China Sea. This is the first time that the compound has been obtained from a marine natural product.



The title molecule is shown in Fig. 1. It lies on a crystallographic center of symmetry and the dihedral angle formed by the planes through the benzene and benzyloxy groups is 61.99 (3)°. The bond lengths and angles (listed in Table 1) are usual for this type of molecule.

In the crystal structure, there are no significant π – π stacking interactions or $\text{C}-\text{H} \cdots \pi(\text{ring})$ interactions and the molecules pack with normal van der Waals separations.

Experimental

The chopped algae were extracted with EtOH at room temperature and then partitioned between EtOAc and H_2O . The resulting organic layer was chromatographed twice on a silica-gel column, yielding the title compound. A sample was dissolved in a mixture of hexane/ether/acetic acid (81.7/18/0.3) at room temperature and normal pressure, and crystals grew over a period of two weeks when the solution was exposed to the air.

Crystal data

$\text{C}_{20}\text{H}_{18}\text{O}_2$
 $M_r = 290.34$
Monoclinic, $P2_1/c$
 $a = 17.565$ (5) Å
 $b = 5.6820$ (17) Å
 $c = 7.804$ (2) Å
 $\beta = 97.622$ (6)°
 $V = 772.0$ (4) Å³
 $Z = 2$

$D_x = 1.249$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 25
reflections
 $\theta = 12$ – 18 °
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
Block, colorless
 $0.29 \times 0.20 \times 0.11$ mm

Data collection

Bruker SMART CCD
diffractometer
 ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.977$, $T_{\max} = 0.991$
4597 measured reflections

1686 independent reflections
1103 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 27.0$ °
 $h = -21 \rightarrow 22$
 $k = -7 \rightarrow 7$
 $l = -6 \rightarrow 9$

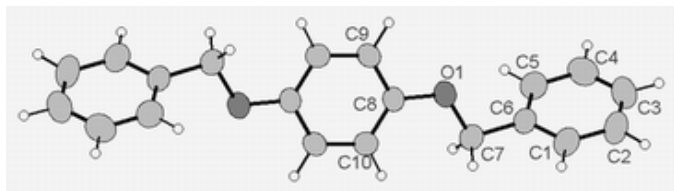


Figure 1
View of the title molecule, showing ellipsoids at the 50% probability level. Unlabeled atoms are related by the symmetry operator $(-x, 1 - y, 1 - z)$.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.138$
 $S = 1.08$
 1686 reflections
 137 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.16 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.036 (8)

Table 1

Selected bond lengths (\AA).

O1—C8	1.3756 (18)	C4—C5	1.380 (3)
O1—C7	1.4253 (19)	C5—C6	1.388 (2)
C1—C2	1.380 (2)	C6—C7	1.499 (2)
C1—C6	1.383 (2)	C8—C9	1.381 (2)
C2—C3	1.371 (3)	C8—C10	1.382 (2)
C3—C4	1.374 (3)	C9—C10 ⁱ	1.386 (2)

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

The H atoms were refined independently with isotropic displacement parameters. The final C—H distances are in the range 0.974 (17)–1.023 (18) \AA .

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine

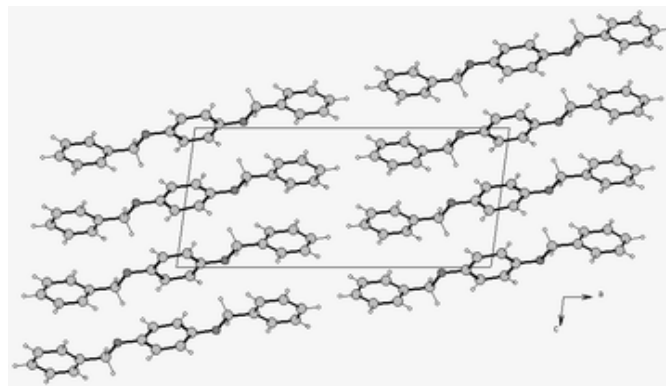


Figure 2
Packing structure of the title compound, viewed along [010].

structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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References

- Bruker (1999). *SAINT* (Version 6.02a) and *SMART* (Version 5.611). Bruker AXS Inc., Madison, Wisconsin, USA.
 McArdle, P. (1995). *ORTEX*. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Zaslow, B. & Dubchansky, J. L. (1967). *Mol. Cryst.* **3**, 297–298.