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2,3,6,7-Tetrahydrobenzo[1,2-*b*;4,5-*b*′]difuran

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.113
Data-to-parameter ratio = 15.9

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

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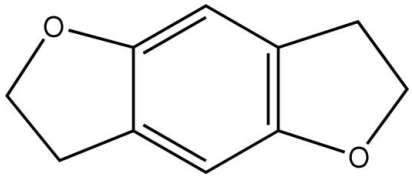
In the crystal structure of the title compound, $C_{10}H_{10}O_2$, the molecule has crystallographic inversion symmetry. Each dihydrofuran ring adopts an envelope conformation and, excluding the flap C atom, is essentially coplanar with the benzene ring.

Comment

Dihydrofurans are an important class of heterocycles with widespread occurrence in nature. Possessing a variety of biological activities, they are used as pharmaceuticals, flavours, insecticides and fish antifeedant agents (Dean, 1982).



(I)

The title compound, (I), crystallizes with half a molecule in the asymmetric unit, the molecule lying on an inversion centre. All bond lengths and angles lie within their expected ranges (Allen *et al.*, 1987). Each dihydrofuran ring adopts an envelope conformation, with atom C1 deviating by 0.190 (2) Å from the mean plane through the other four atoms. This mean plane forms a dihedral angle of 0.32 (6)° with the benzene ring.

There are no π–π stacking interactions in the crystal structure of (I). The packing is shown in Fig. 2.

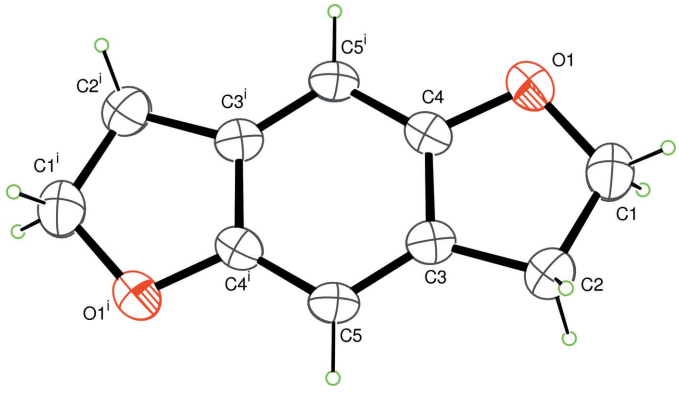


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small circles of arbitary radii. [Symmetry code: (i) 1 − *x*, 1 − *y*, 1 − *z*.]

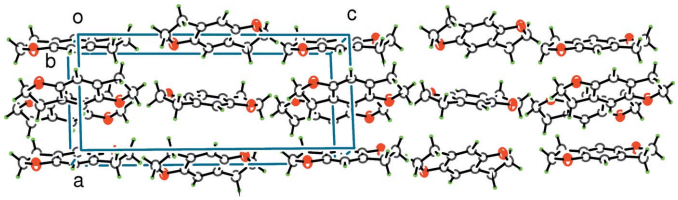


Figure 2
The molecular packing of (I).

Experimental

1,4-Dibromo-2,5-bis(2-chloroethoxy)benzene (3.93 g, 10 mmol) was dissolved in dry tetrahydrofuran (100 ml) in a nitrogen atmosphere and cooled to 273 K. A solution of 2.0 *M* *n*-butyllithium (5.5 ml, 11 mmol) was added quickly. The mixture was stirred at room temperature for 10 min, then extracted with diethyl ether and water, dried with anhydrous $MgSO_4$, and the solid product recrystallized from diethyl ether to obtain the title compound (0.98 g, yield 60%) (Monte *et al.*, 1996). It was further recrystallized from acetone, giving colourless crystals suitable for X-ray diffraction.

Crystal data

$C_{10}H_{10}O_2$
$M_r = 162.19$
Orthorhombic, *Pbca*
$a = 7.434\ (4)$ Å
$b = 5.972\ (2)$ Å
$c = 17.603\ (9)$ Å
$V = 781.4\ (6)$ Å^3
$Z = 4$
$D_x = 1.378$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5940 reflections
$\theta = 3.4$–$27.5°$
$\mu = 0.10$ mm^{-1}
$T = 296\ (1)$ K
Block, colourless
0.36 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
6952 measured reflections
891 independent reflections
656 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 7$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.113$
$S = 1.02$
891 reflections
56 parameters
H-atom parameters constrained
$w = 1/[0.0012F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 2.7 (4) × 10^2

H atoms were placed in idealized positions (C—H = 0.93–0.97 Å) and refined as riding on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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