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(*S*)-3,3′-Dibromo-5,5′,6,6′,7,7′,8,8′-octahydro-2,2′-dimethoxy-1,1′-binaphthalene

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The title compound, $C_{22}H_{24}Br_2O_2$, consists of two substituted tetralin units that are connected through a C—C single bond; the aromatic rings are twisted by 80.2 (2)°.

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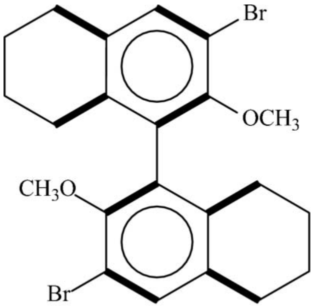
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.114
Data-to-parameter ratio = 17.9

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

Comment

Crystal structures of chiral organic compounds that differ only in their absolute configurations are not normally reported, probably because no large differences in bond dimensions are expected between them. The title chiral bi-tetralin derivative, (I), is the *S*-isomer of the Brönsted acid that catalyses asymmetric Morita–Baylis–Hillman reactions (He & Ng, 2006) (Fig. 1). This isomer exhibits disorder in only one alicyclic ring, unlike the *R*-isomer, which is disordered in both rings. The compound also has a somewhat larger cell volume compared with that [1956.1 (1) Å^3] of the *R* isomer.



(I)

Experimental

Crystals of the title compound were obtained by using a modification of a literature procedure, with optically active (*S*)-1,1′-binaphthalene-2,2′-diol [(*S*)-BINOL] as the starting reactant (He & Ng, 2006) in place of (*R*)-BINOL. Crystals were grown from a dichloromethane solution of the compound.

Crystal data

$C_{22}H_{24}Br_2O_2$
M_r = 480.23
Orthorhombic, $P2_12_12_1$
a = 10.004 (1) Å
b = 12.086 (1) Å
c = 17.434 (2) Å
V = 2107.9 (4) Å^3
Z = 4
D_x = 1.513 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.86 mm^{-1}
T = 295 (2) K
Block, colourless
0.26 × 0.20 × 0.12 mm

Data collection

Bruker SMART 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.434, $T_{\max}$ = 0.655
11804 measured reflections
4338 independent reflections
2993 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.051
$\theta_{\max}$ = 26.5°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.114$	$\Delta\rho_{max} = 0.61$ e Å^{-3}
$S = 0.96$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
4338 reflections	Absolute structure: Flack (1983), with 1858 Friedel pairs
242 parameters	Flack parameter: −0.01 (2)
H-atom parameters constrained	

The alicyclic ring of one of the two tetralin units is disordered over two sites; the atoms involved are C8, C9 with their attached H atoms, and also the H atoms attached to C7 and C10. Site occupancy factors refined to 0.63 (1):0.37 (1). For both aromatic rings,, the C—C distances were restrained to 1.390 (5) Å. For the alicyclic rings, these were restrained to 1.500 (1) Å; additionally, the 1,3-related distances were restrained to 2.45 (1) Å. The displacement parameters of the primed atoms were set equal to those of the unprimed atoms. Atoms C18 and C19 display elongated ellipsoids, suggesting the presence of disorder, but no reliable disorder model could be produced. C-bound H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2006).

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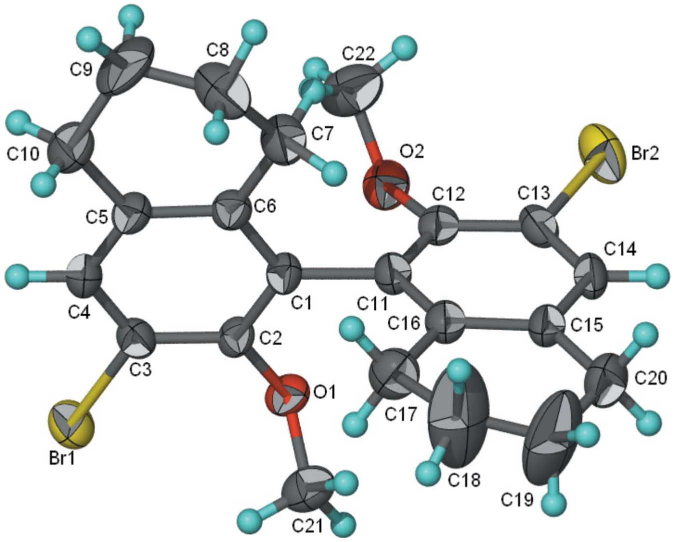

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius. Only the major disorder component is shown.

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