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(1*RS*,2*SR*)-1,2,4,5,7-Pentabromo-5-methoxyindane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.041
wR factor = 0.073
Data-to-parameter ratio = 24.4

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

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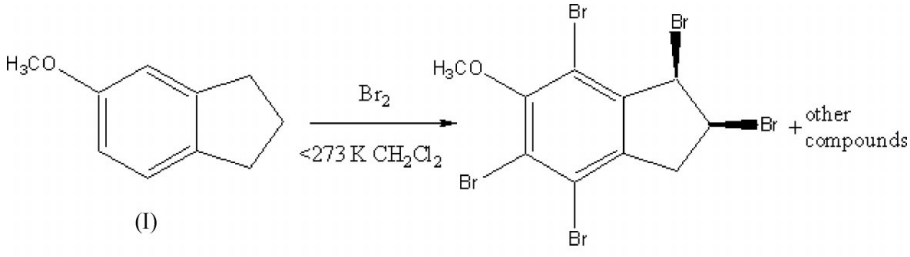
In the title compound, $C_{10}H_7Br_5O$, prepared by bromination of 5-methoxyindane, all bond lengths and angles are in the usual ranges. However, the relatively wide range of Br—C—C angles [107.2 (5)–117.0 (4)°] in the five-membered ring may indicate repulsion between the neighbouring Br atoms. The crystal packing is stabilized by van der Waals interactions.

Comment

Indanes are present in a large number of natural products and in compounds of pharmaceutical importance (Quiclet-Sire *et al.*, 1999, and references therein). Indane-derived chiral ligands have also found application in transition metal-catalyzed processes (Zhang *et al.*, 2003, and references therein). Bromination of hydrocarbons often leads to useful intermediates used in the synthesis of bromoorganic compounds. These materials have numerous industrial applications as pesticides, plastics, fire retardants and pharmaceutical chemicals (Hileman, 1993). Bromoindanes are important key intermediates in the industrial and laboratory preparation of hydroxy and epoxide compounds (Crosman *et al.*, 2004), and of indenone and fluorenone compounds (Tutar *et al.*, 2001).



(I) (II)

In the title compound, (II) (Fig. 1), prepared by bromination of 5-methoxyindane, (I), all bond lengths and angles (Table 1) are in the usual ranges observed in related structures (Allen *et al.*, 1987; Çelik *et al.*, 2002; Hökelek *et al.*, 1990, 1991, 1998; Akkurt *et al.*, 2004). The five-membered ring adopts the envelope conformation, with puckering parameters (Cremer & Pople, 1975) Q_2 = 0.309 (8) Å and φ_2 = 70.5 (15)°. The five Br—C distances in (II) range from 1.884 (7) to 1.980 (7) Å. The relatively wide range of Br—C—C angles [107.2 (5)–117.0 (4)°] in the five-membered ring may indicate repulsion between the neighbouring Br atoms.

There are no unusual short contacts between the molecules in (II). The crystal packing (Fig. 2) is stabilized by van der Waals interactions.

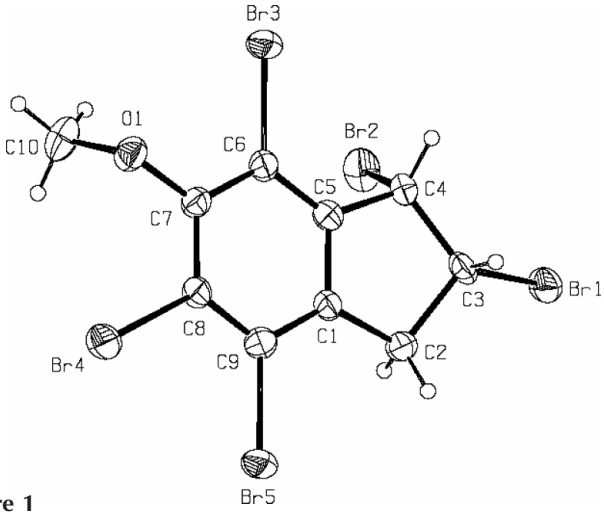


Figure 1
The molecular structure of (II). Displacement ellipsoids are drawn at the 50% probability level.

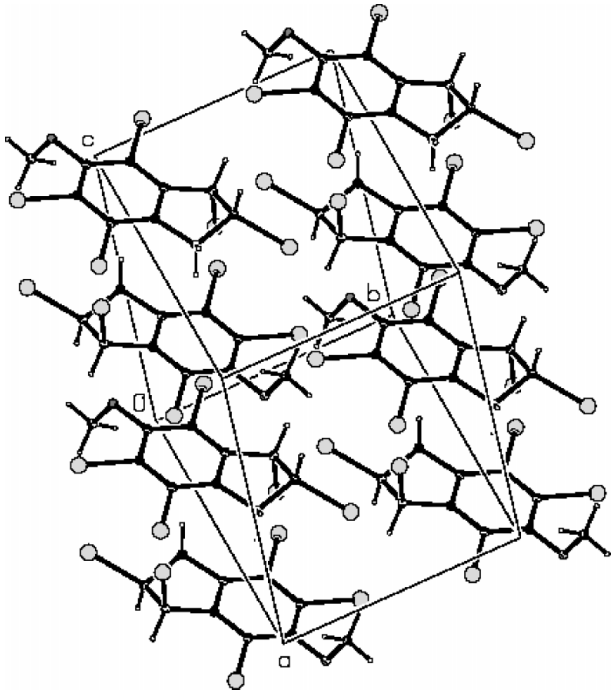


Figure 2
Packing diagram of (II), viewed approximately along [101].

Experimental

The title compound was prepared by bromination of 5-methoxyindane according to the following procedure. An excess of bromine was added to a solution of 5-methoxyindane in CH_2Cl_2 at below 273 K and allowed to stand for three weeks in a refrigerator. The reaction progress was monitored by thin-layer chromatography. After consumption of 5-methoxyindane, the excess bromine and solvent were removed at reduced pressure and at 293 K. The residue was crystallized from hexane–dichloromethane (1:5, 12 ml) at room temperature over a period of 1 d to give colourless block-like crystals (yield: 18%, m.p. 458–460 K).

Crystal data

$C_{10}H_7Br_5O$	$Z = 2$
$M_r = 542.66$	$D_x = 2.682$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo Kα radiation
$a = 8.8895$ (11) Å	Cell parameters from 7984 reflections
$b = 8.9281$ (10) Å	$\theta = 2.4$–$29.5°$
$c = 9.6787$ (13) Å	$\mu = 14.93$ mm^{-1}
$\alpha = 98.382$ (10)°	$T = 293$ K
$\beta = 113.160$ (10)°	Block, colourless
$\gamma = 101.060$ (9)°	0.55 × 0.41 × 0.26 mm
$V = 671.99$ (16) Å^3	

Data collection

Stoe IPDS-II diffractometer	3563 independent reflections
ω scans	1562 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)	$R_{int} = 0.167$
	$\theta_{max} = 29.6°$
	$h = -12 \rightarrow 11$
$T_{min} = 0.045$, $T_{max} = 0.112$	$k = -12 \rightarrow 12$
13 393 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.074$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
$S = 0.81$	$\Delta\rho_{min} = -0.67$ e Å^{-3}
3563 reflections	Extinction correction: *SHELXL*97
146 parameters	Extinction coefficient: 0.0076 (5)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Br1—C3	1.930 (7)	Br5—C9	1.884 (7)
Br2—C4	1.980 (7)	O1—C7	1.368 (9)
Br3—C6	1.889 (7)	O1—C10	1.445 (10)
Br4—C8	1.889 (6)		
C7—O1—C10	112.5 (6)	O1—C7—C6	122.2 (6)
Br1—C3—C2	112.9 (5)	O1—C7—C8	120.3 (6)
Br1—C3—C4	117.0 (4)	Br4—C8—C7	117.2 (5)
Br2—C4—C3	112.6 (5)	Br4—C8—C9	120.8 (5)
Br2—C4—C5	107.2 (5)	Br5—C9—C1	118.1 (6)
Br3—C6—C5	121.1 (5)	Br5—C9—C8	122.2 (5)
Br3—C6—C7	117.9 (6)		

H atoms were geometrically positioned and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2–1.5U_{eq}(C)] using a riding model, with C—H = 0.98 (CH), 0.97 (CH_2) and 0.96 Å (CH_3).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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