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1-(2,2-Dibromovinyl)-3,5-dimethoxybenzene

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Key indicators

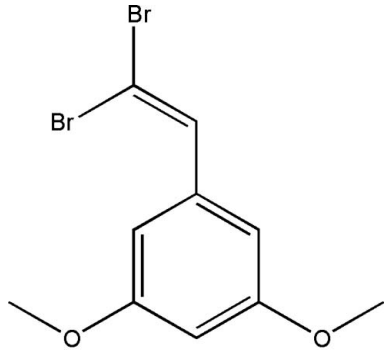
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.015 Å
R factor = 0.065
wR factor = 0.194
Data-to-parameter ratio = 16.1

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

In the title compound, $C_{10}H_{10}Br_2O_2$, the angle between the dibromovinyl group and the benzene ring is 42.2 (2)°.

Comment

The title compound, (I), is a vinylic dibromide derivative prepared from 3,5-dimethoxybenzaldehyde (Papahatjis *et al.*, 1998) and its structure is presented here (Fig. 1).



(I)

In styrene, both the benzene ring and the double bond are coplanar due to conjugation. This is not possible in the case of (I) due to steric repulsion between the vinylic Br atom and benzene CH moieties.The double bond and the benzene ring of the title compound are inclinhed at a dihedral angle of 42.2 (2)°.

Experimental

The title compound was prepared according to the procedure of Papahatjis *et al.* (1998). Suitable crystals were obtained by evaporation of an ethyl acetate/hexane (1:4 *v*/*v*) solution (m.p. 345 K).

Crystal data

$C_{10}H_{10}Br_2O_2$
M_r = 321.98
Monoclinic, $P2_1/n$
a = 4.129 (2) Å
b = 11.192 (6) Å
c = 25.732 (15) Å
β = 92.274 (10)°
V = 1188.2 (11) Å^3
Z = 4
D_x = 1.800 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.80 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.24 × 0.12 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.186, T_{max} = 0.442
5582 measured reflections
2086 independent reflections
1422 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.0°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 5.9795P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.066$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.194$	$\Delta\rho_{max} = 1.00$ e Å^{-3}
$S = 1.18$	$\Delta\rho_{min} = -0.82$ e Å^{-3}
2086 reflections	Extinction correction: *SHELXL*
130 parameters	Extinction coefficient: 0.013 (2)
H-atom parameters constrained	

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.96 Å); for the CH and CH_2 groups, U_{iso}(H) values were set equal to $1.2U_{eq}$(C), and $1.5U_{eq}$(C) for the methyl groups.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Molecular Structure Corporation & Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure*.

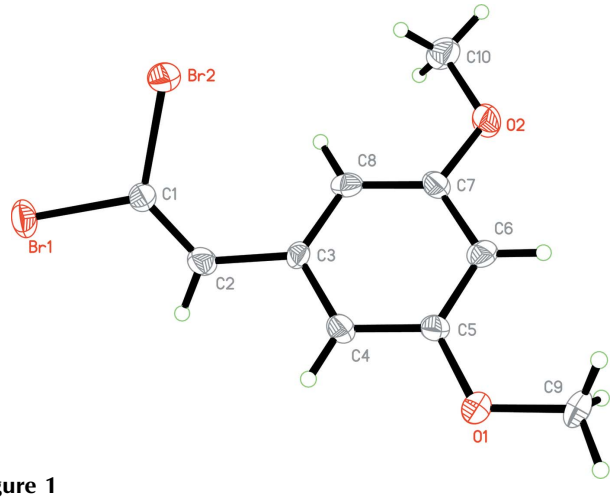


Figure 1
The molecular structure of (I), with the atom numbering scheme, showing displacement ellipsoids drawn at the 35% probability level.

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