Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3-Bis(bromomethyl)-1,4-dimethoxybenzene

Peter Hammershøj and Jørn B. Christensen*

University of Copenhagen, Department of Chemistry, Universitetsparken 5, DK-2100 Copenhagen, Denmark

Correspondence e-mail: jbc@kiku.dk

Key indicators

Single-crystal X-ray study
T = 122 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.063
Data-to-parameter ratio = 32.9

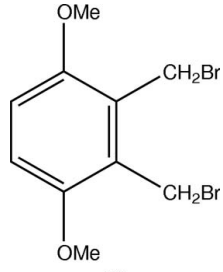
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{10}H_{12}Br_2O_2$, all bond lengths and angles are generally within the normal ranges. The crystal packing is stabilized mainly by van der Waals forces.

Received 6 July 2005
Accepted 4 August 2005
Online 12 August 2005

Comment

The title compound, (I) (Fig. 1), was prepared for use as a building block in the syntheses of Single-walled Carbon Nanotube (SWNT) interacting compounds. In (I), the bond lengths and angles (Table 1) are generally within the normal ranges. The two methoxy groups are slightly out of the plane of benzene ring having C3—C4—O1—C7 and C8—O2—C1—C2 torsion angles of 175.15 (17) and 173.40 (17)°, respectively. The bromomethyl groups are almost perpendicular to the benzene ring, with Br1—C9—C3—C4 and Br2—C10—C2—C1 torsion angles of −79.57 (19) and 97.29 (17)°, respectively. The crystal packing is stabilized mainly by van der Waals forces.



(I)

Experimental

The title compound was prepared according to the procedure of Eskildsen *et al.* (2000). Crystals suitable for X-ray analysis were prepared by crystallization from ethanol.

Crystal data

$C_{10}H_{12}Br_2O_2$
M_r = 324.01
Triclinic, $P\overline{1}$
a = 4.4740 (8) Å
b = 7.6630 (8) Å
c = 16.463 (2) Å
α = 94.685 (11)°
β = 94.945 (9)°
γ = 98.276 (13)°
V = 553.93 (14) Å^3
Z = 2
D_x = 1.943 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13534 reflections
θ = 1.3–33.0°
μ = 7.29 mm^{-1}
T = 122 (2) K
Needle, white
0.53 × 0.16 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω and φ scans
Absorption correction: integration via Gaussian integration (Coppens, 1970)
T_{min} = 0.149, T_{max} = 0.865
23530 measured reflections
4180 independent reflections
3390 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 33.0°
$h = -6 \rightarrow 6$
$k = -11 \rightarrow 11$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0164P)^2 + 0.629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.063$	$\Delta\rho_{max} = 0.64$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.49$ e Å^{-3}
4180 reflections	
127 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Br1—C9	1.9776 (19)	C2—C10	1.492 (3)
Br2—C10	1.987 (2)	C1—C6	1.384 (3)
C3—C2	1.398 (3)	C6—C5	1.391 (3)
C3—C4	1.406 (3)	C6—H6	0.9500
C3—C9	1.493 (3)	C5—C4	1.389 (3)
O2—C1	1.375 (2)	O1—C4	1.367 (2)
O2—C8	1.431 (2)	O1—C7	1.429 (3)
C2—C1	1.411 (3)		
C2—C3—C4	119.31 (17)	O2—C1—C6	123.88 (17)
C2—C3—C9	122.37 (17)	C6—C1—C2	120.35 (17)
C4—C3—C9	118.31 (17)	C1—C6—C5	120.22 (18)
C3—C2—C1	119.53 (17)	C4—C5—C6	119.98 (17)
C3—C2—C10	122.28 (17)	C5—C4—C3	120.60 (17)

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

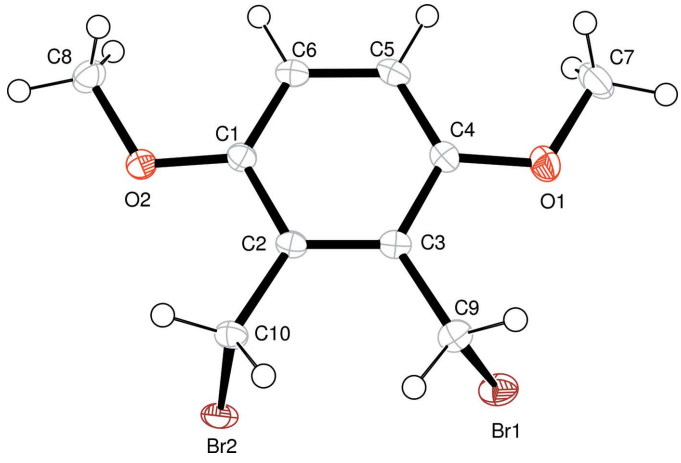


Figure 1
View of (I) with the 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radii.

The authors thank Flemming Hansen for collecting the diffraction data and the Centre for Crystallographic Studies for the use of their equipment.

References

Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Coppens, P. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 255–270. Copenhagen: Munksgaard.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Eskildsen, J., Reenberg, T., Larsen, U. & Christensen, J. B. (2000). *Org. Prep. Proc. Int.* **32**, 398–400.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.