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1,2-Dibromo-4,5-dimethylbenzene

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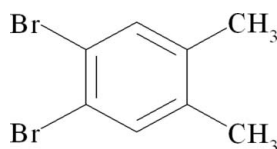
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 18.7.

In the title compound, $\text{C}_8\text{H}_8\text{Br}_2$, the bond lengths and angles are in the normal range. All non-H atoms are coplanar.

Related literature

The structures of the related compounds 1,2-dibromo-4,5-dimethyl-3-nitrobenzene and 1,2-dibromo-4,5,6-trimethyl-3-nitrobenzene have been reported by Skakle *et al.* (2006). For related literature, see: Allen *et al.* (1987); Lawson *et al.* (1968); Stoddart (1989).



Experimental

Crystal data

$\text{C}_8\text{H}_8\text{Br}_2$
 $M_r = 263.96$
 Monoclinic, $P2_1/n$
 $a = 9.383$ (4) Å
 $b = 7.918$ (3) Å
 $c = 12.612$ (5) Å
 $\beta = 109.041$ (6)°

$V = 885.7$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 9.08$ mm⁻¹
 $T = 298$ (2) K
 $0.20 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.264$, $T_{\max} = 0.464$
 (expected range = 0.230–0.403)

4542 measured reflections
 1735 independent reflections
 1346 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.097$
 $S = 1.07$
 1735 reflections

93 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1994); data reduction: XPREP (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2106).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Lawson, D. W., McOmie, J. F. W. & West, D. E. (1968). *J. Chem. Soc.* pp. 2414–2415.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1994). *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *XPREP*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Skakle, J. M. S., Gojdka, B. & Wardell, J. L. (2006). *Acta Cryst.* **E62**, o1001–o1002.
- Stoddart, J. F. (1989). *Annu. Rep. Prog. Chem. Sect. B*, **86**, 353–387.

supplementary materials

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1,2-Dibromo-4,5-dimethylbenzene

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Comment

Molecules which possess novel belt-like and cage-like structures have played a central role in the development of supramolecular chemistry (Stoddart, 1989). Since maleimide derivatives are used frequently as the dienophiles in Diels-Alder cycloadditions, we are investigating methods of incorporating the maleimide moiety into 2-amino-1,2,3-triazolequinone derivatives. Considering the strategy synthetic in where the compound (I) it is used like precursor, we report here the structure of (I), Fig.1.

Experimental

The title compound was synthesized according to a method described previously (Lawson *et al.*, 1968). The reaction solution was diluted with diethyl ether and washed with brine. The organic solution was dried over MgSO_4 and the solvent removed. Recrystallization in MeOH to give product as white crystals. $^1\text{H-NMR}$ (300 MHz, CDCl_3): (p.p.m.) = 7.35 (s, 2H), 2.17 (s, 6H). Analysis calculated for $\text{C}_8\text{H}_8\text{Br}_2$: C 36.40, H 3.05; found (%): C 35.92, H 3.38.

Refinement

The structure was solved by direct methods. All H atoms were placed at geometrically idealized positions and were treated as riding atoms, with $\text{C-H} = 0.93 \text{ \AA}$ (aromatic) or 0.96 \AA (methyl), and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ for aromatic and $1.5U_{\text{eq}}$ for methyl H atoms.

Figures

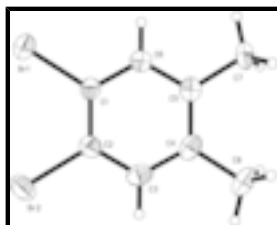


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

1,2-Dibromo-4,5-dimethylbenzene

Crystal data

$\text{C}_8\text{H}_8\text{Br}_2$

$M_r = 263.96$

Monoclinic, $P2_1/n$

$F_{000} = 504$

$D_x = 1.980 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: -P2yn

$a = 9.383 (4) \text{ \AA}$

$b = 7.918 (3) \text{ \AA}$

$c = 12.612 (5) \text{ \AA}$

$\beta = 109.041 (6)^\circ$

$V = 885.7 (6) \text{ \AA}^3$

$Z = 4$

Cell parameters from 1764 reflections

$\theta = 2.4\text{--}25.1^\circ$

$\mu = 9.08 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Block, white

$0.20 \times 0.12 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

ω scans

Absorption correction: empirical (using intensity
measurements)

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.264$, $T_{\max} = 0.464$

4542 measured reflections

1735 independent reflections

1346 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.4^\circ$

$h = -8 \rightarrow 11$

$k = -7 \rightarrow 9$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.097$

$S = 1.07$

1735 reflections

93 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.5399P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	-0.20495 (5)	0.21958 (7)	0.68821 (4)	0.0680 (2)
Br2	0.06751 (6)	0.44884 (7)	0.87503 (4)	0.0710 (2)
C3	0.2076 (5)	0.4319 (5)	0.7077 (4)	0.0524 (11)
H3	0.2817	0.4961	0.7588	0.063*
C1	-0.0297 (4)	0.2898 (5)	0.6581 (3)	0.0445 (9)
C2	0.0831 (5)	0.3833 (5)	0.7341 (3)	0.0460 (9)
C5	0.1127 (5)	0.2935 (5)	0.5291 (4)	0.0473 (10)
C4	0.2257 (5)	0.3871 (5)	0.6057 (4)	0.0513 (10)
C6	-0.0124 (5)	0.2452 (5)	0.5561 (3)	0.0481 (10)
H6	-0.0870	0.1814	0.5051	0.058*
C8	0.3680 (6)	0.4447 (6)	0.5815 (5)	0.0670 (13)
H8A	0.3400	0.5149	0.5159	0.101*
H8B	0.4219	0.3476	0.5691	0.101*
H8C	0.4312	0.5075	0.6444	0.101*
C7	0.1231 (6)	0.2415 (6)	0.4139 (4)	0.0561 (11)
H7A	0.2090	0.1695	0.4246	0.084*
H7B	0.1336	0.3406	0.3732	0.084*
H7C	0.0332	0.1819	0.3721	0.084*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0524 (3)	0.0926 (4)	0.0663 (3)	-0.0102 (2)	0.0294 (2)	-0.0049 (3)
Br2	0.0788 (4)	0.0802 (4)	0.0534 (3)	0.0011 (3)	0.0206 (3)	-0.0182 (2)
C3	0.043 (2)	0.044 (2)	0.063 (3)	0.0005 (18)	0.008 (2)	0.0017 (19)
C1	0.041 (2)	0.047 (2)	0.048 (2)	0.0053 (17)	0.0171 (18)	0.0016 (17)
C2	0.046 (2)	0.045 (2)	0.044 (2)	0.0071 (18)	0.0109 (18)	-0.0016 (17)
C5	0.051 (2)	0.043 (2)	0.051 (2)	0.0062 (19)	0.0201 (19)	0.0062 (18)
C4	0.043 (2)	0.043 (2)	0.072 (3)	0.0071 (18)	0.025 (2)	0.010 (2)
C6	0.047 (2)	0.051 (2)	0.046 (2)	-0.0028 (18)	0.0147 (19)	-0.0035 (17)
C8	0.055 (3)	0.062 (3)	0.095 (4)	-0.006 (2)	0.040 (3)	0.013 (3)
C7	0.064 (3)	0.068 (3)	0.048 (2)	0.006 (2)	0.034 (2)	0.008 (2)

Geometric parameters (\AA , $^\circ$)

Br1—C1	1.889 (4)	C5—C7	1.544 (6)
Br2—C2	1.902 (4)	C4—C8	1.532 (6)
C3—C2	1.371 (6)	C6—H6	0.9300
C3—C4	1.398 (6)	C8—H8A	0.9600
C3—H3	0.9300	C8—H8B	0.9600
C1—C2	1.387 (6)	C8—H8C	0.9600
C1—C6	1.393 (6)	C7—H7A	0.9600
C5—C6	1.380 (6)	C7—H7B	0.9600
C5—C4	1.392 (6)	C7—H7C	0.9600

supplementary materials

C2—C3—C4	121.5 (4)	C5—C6—C1	121.5 (4)
C2—C3—H3	119.3	C5—C6—H6	119.2
C4—C3—H3	119.3	C1—C6—H6	119.2
C2—C1—C6	118.8 (4)	C4—C8—H8A	109.5
C2—C1—Br1	122.4 (3)	C4—C8—H8B	109.5
C6—C1—Br1	118.8 (3)	H8A—C8—H8B	109.5
C3—C2—C1	120.0 (4)	C4—C8—H8C	109.5
C3—C2—Br2	118.8 (3)	H8A—C8—H8C	109.5
C1—C2—Br2	121.2 (3)	H8B—C8—H8C	109.5
C6—C5—C4	119.5 (4)	C5—C7—H7A	109.5
C6—C5—C7	118.6 (4)	C5—C7—H7B	109.5
C4—C5—C7	121.9 (4)	H7A—C7—H7B	109.5
C5—C4—C3	118.7 (4)	C5—C7—H7C	109.5
C5—C4—C8	122.4 (4)	H7A—C7—H7C	109.5
C3—C4—C8	118.9 (4)	H7B—C7—H7C	109.5

Fig. 1

