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1-Bromoadamantane

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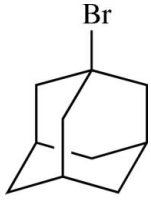
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.007 Å; R factor = 0.032; wR factor = 0.080; data-to-parameter ratio = 16.1.

The molecule of the title compound, $C_{10}H_{15}Br$, shows noncrystallographic mirror symmetry. In the crystal structure, no intermolecular interactions with distances less than the sum of the van der Waals radii of the respective atoms are present.

Related literature

For the crystal structure of the thiourea solvate of the compound, see Chao *et al.* (2003).



Experimental

Crystal data

$C_{10}H_{15}Br$ M_r = 215.13
Monoclinic, $P2_1/c$
a = 10.154 (3) Å
b = 6.8541 (11) Å
c = 13.240 (3) Å
β = 90.027 (17)°
V = 921.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.40 mm^{-1}
T = 200 (2) K
0.21 × 0.16 × 0.13 mm

Data collection

Oxford Xcalibur diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.462, T_{max} = 0.614
4563 measured reflections
1629 independent reflections
1313 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.02
1629 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Professor Dr Klapötke is thanked for generous allocation of measurement time on the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2442).

References

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Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o101 [doi:10.1107/S1600536808038452]

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S1. Comment

The structure of the title compound was elucidated for comparison of the influence of different substituents on the geometry of the adamantane framework.

In the molecule the Br atom is bonded to one of the bridgehead positions of the carbocycle (Fig. 1). Bond lengths are normal.

In the crystal structure, only dispersive interactions are present. No intermolecular contacts whose range falls below the sum of the van der Waals radii of the respective atoms are existent.

A similar structure, the thiourea solvate of the compound, has been described by Chao *et al.* (2003) but showed disorder among the 1-bromoadamantane moiety. However, a comparison of both molecules shows good agreement in terms of bond lengths and angles.

The packing of the compound is shown in Fig. 2.

S2. Experimental

The compound was obtained commercially (ACROS). Crystals suitable for X-ray analysis were obtained upon free evaporation of a solution of the compound in diethyl ether.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.99 Å for methylene groups and C—H 1.00 Å for bridgehead positions) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

The crystal measured is refined as a twin with a twin-plane perpendicular to [001] (*Ebenenzwilling*). The volume-to-volume-ratio for the two individuals is found at approximately 1:1 with a batch-scale factor of approximately 0.46.

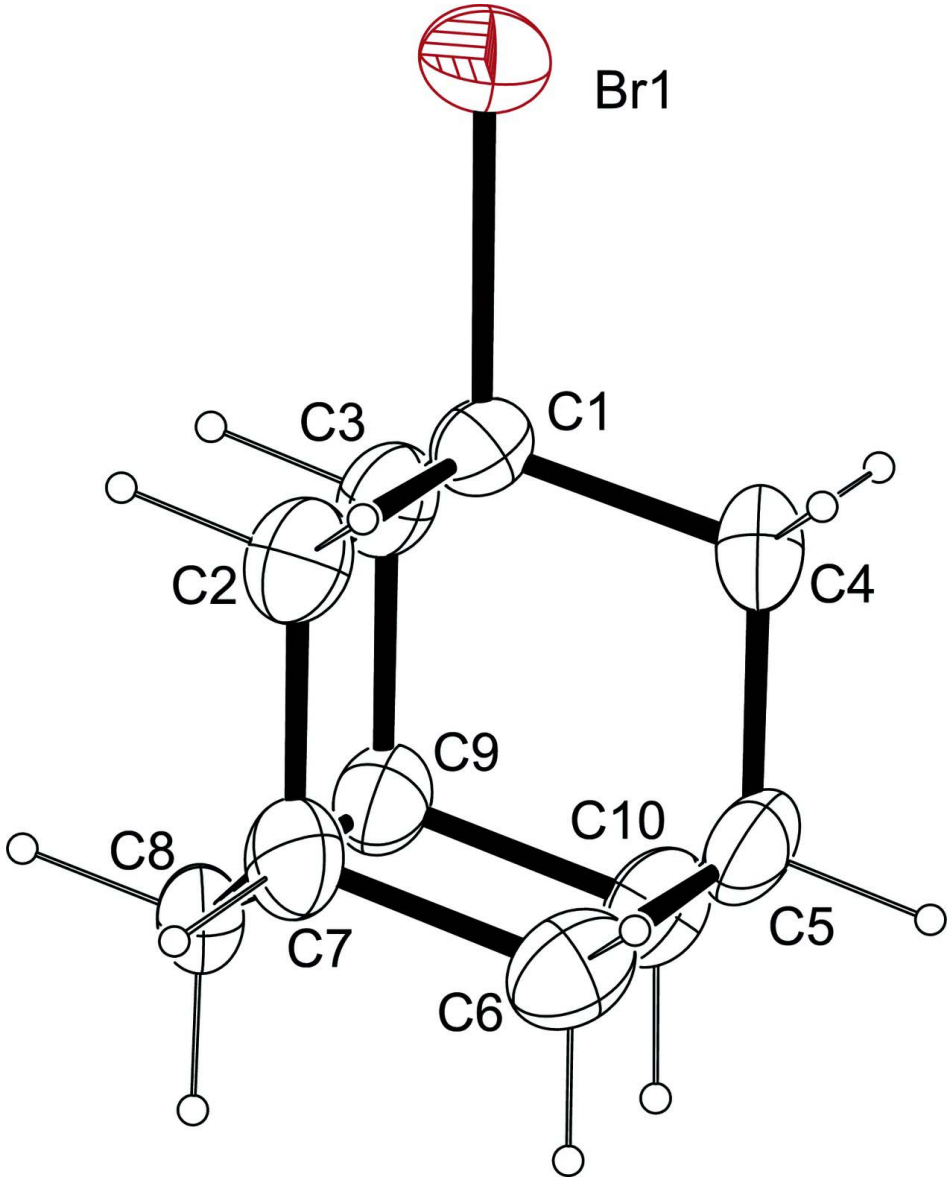

Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

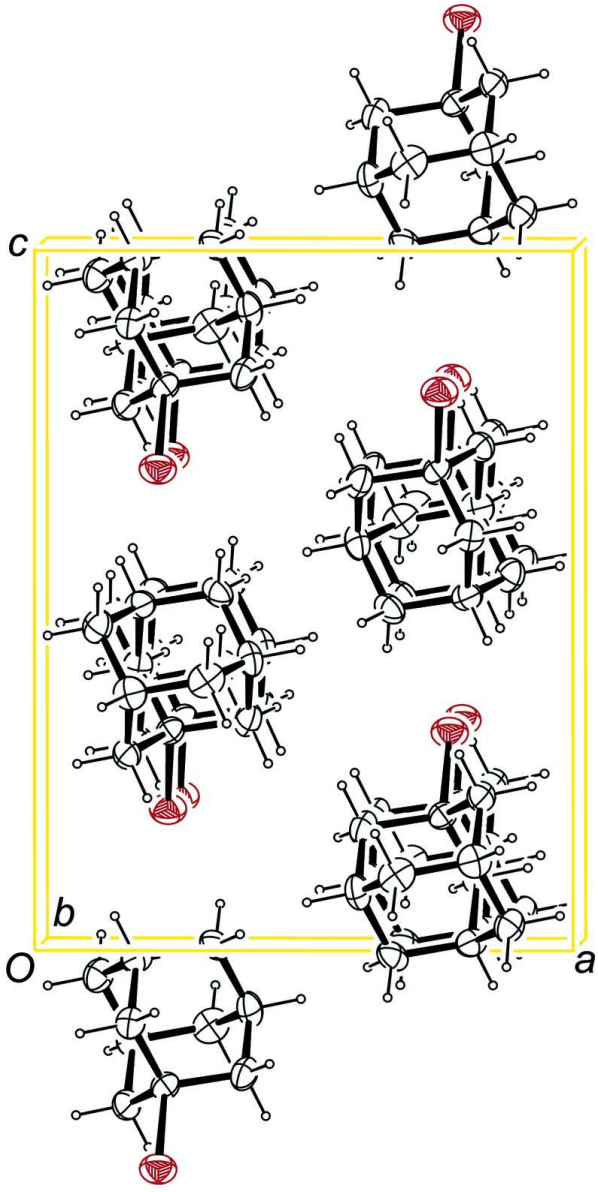

Figure 2

The packing of the title compound, viewed along [010].

1-Bromoadamantane

Crystal data

$C_{10}H_{15}Br$
$M_r = 215.13$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.154\ (3)$ Å
$b = 6.8541\ (11)$ Å
$c = 13.240\ (3)$ Å
$\beta = 90.027\ (17)°$
$V = 921.5\ (4)$ Å^3
$Z = 4$

$F(000) = 440$
$D_x = 1.551$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2345 reflections
$\theta = 3.9–26.3°$
$\mu = 4.40$ mm^{-1}
$T = 200$ K
Block, colourless
0.21 × 0.16 × 0.13 mm

Data collection

Oxford Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.462, T_{max} = 0.614
4563 measured reflections
1629 independent reflections
1313 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.3°, θ_{min} = 3.9°
h = −12→11
k = −8→8
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.02
1629 reflections
101 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.23244 (6)	0.64478 (6)	0.19046 (4)	0.04391 (18)
C1	0.2412 (4)	0.4548 (6)	0.3057 (3)	0.0281 (9)
C2	0.3872 (4)	0.4075 (6)	0.3225 (4)	0.0361 (11)
H21	0.4369	0.5279	0.3386	0.043*
H22	0.4255	0.3481	0.2610	0.043*
C3	0.1789 (4)	0.5508 (7)	0.3973 (3)	0.0315 (11)
H31	0.0859	0.5840	0.3829	0.038*
H32	0.2266	0.6724	0.4144	0.038*
C4	0.1651 (5)	0.2707 (7)	0.2754 (3)	0.0330 (11)
H41	0.2042	0.2120	0.2140	0.040*
H42	0.0719	0.3031	0.2612	0.040*
C5	0.1743 (6)	0.1266 (7)	0.3651 (4)	0.0356 (14)
H5	0.1251	0.0048	0.3477	0.043*
C6	0.3174 (6)	0.0759 (8)	0.3849 (5)	0.0418 (15)
H61	0.3563	0.0147	0.3241	0.050*
H62	0.3233	−0.0185	0.4413	0.050*
C7	0.3940 (4)	0.2628 (8)	0.4118 (4)	0.0372 (13)
H7	0.4880	0.2294	0.4261	0.045*
C8	0.3321 (6)	0.3549 (7)	0.5051 (4)	0.0345 (14)
H81	0.3807	0.4752	0.5229	0.041*
H82	0.3390	0.2633	0.5627	0.041*
C9	0.1869 (6)	0.4047 (7)	0.4865 (4)	0.0317 (13)
H9	0.1480	0.4648	0.5486	0.038*
C10	0.1118 (5)	0.2199 (8)	0.4592 (4)	0.0369 (13)
H101	0.0184	0.2519	0.4454	0.044*

H102	0.1149	0.1268	0.5163	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0506 (3)	0.0472 (3)	0.0339 (2)	−0.0028 (3)	−0.0007 (3)	0.0092 (2)
C1	0.030 (2)	0.0264 (19)	0.0282 (19)	−0.0018 (18)	0.003 (4)	0.0013 (18)
C2	0.027 (2)	0.040 (3)	0.042 (3)	−0.006 (2)	0.007 (2)	−0.002 (2)
C3	0.031 (3)	0.026 (2)	0.037 (3)	0.000 (2)	0.001 (2)	−0.005 (2)
C4	0.029 (2)	0.037 (3)	0.033 (2)	−0.008 (2)	−0.001 (2)	−0.009 (2)
C5	0.042 (3)	0.023 (3)	0.042 (3)	−0.010 (2)	0.000 (3)	−0.003 (2)
C6	0.050 (4)	0.029 (3)	0.046 (3)	0.001 (3)	0.006 (3)	−0.002 (3)
C7	0.024 (2)	0.040 (3)	0.048 (4)	−0.006 (3)	−0.005 (2)	0.002 (3)
C8	0.035 (3)	0.036 (3)	0.033 (3)	−0.012 (3)	−0.009 (2)	0.002 (2)
C9	0.036 (3)	0.031 (3)	0.029 (3)	−0.007 (2)	0.003 (2)	−0.003 (2)
C10	0.033 (3)	0.035 (3)	0.043 (3)	−0.008 (2)	0.004 (3)	0.001 (2)

Geometric parameters (Å, º)

Br1—C1	2.008 (4)	C5—C10	1.538 (8)
C1—C3	1.518 (6)	C5—H5	1.0000
C1—C4	1.533 (6)	C6—C7	1.540 (8)
C1—C2	1.533 (6)	C6—H61	0.9900
C2—C7	1.545 (7)	C6—H62	0.9900
C2—H21	0.9900	C7—C8	1.523 (8)
C2—H22	0.9900	C7—H7	1.0000
C3—C9	1.551 (6)	C8—C9	1.533 (7)
C3—H31	0.9900	C8—H81	0.9900
C3—H32	0.9900	C8—H82	0.9900
C4—C5	1.547 (7)	C9—C10	1.522 (7)
C4—H41	0.9900	C9—H9	1.0000
C4—H42	0.9900	C10—H101	0.9900
C5—C6	1.517 (8)	C10—H102	0.9900
C3—C1—C4	110.8 (4)	C5—C6—C7	109.4 (5)
C3—C1—C2	112.3 (4)	C5—C6—H61	109.8
C4—C1—C2	110.6 (4)	C7—C6—H61	109.8
C3—C1—Br1	107.9 (3)	C5—C6—H62	109.8
C4—C1—Br1	108.2 (3)	C7—C6—H62	109.8
C2—C1—Br1	106.9 (3)	H61—C6—H62	108.2
C1—C2—C7	106.8 (4)	C8—C7—C6	108.9 (4)
C1—C2—H21	110.4	C8—C7—C2	109.6 (4)
C7—C2—H21	110.4	C6—C7—C2	109.6 (4)
C1—C2—H22	110.4	C8—C7—H7	109.6
C7—C2—H22	110.4	C6—C7—H7	109.6
H21—C2—H22	108.6	C2—C7—H7	109.6
C1—C3—C9	107.9 (4)	C7—C8—C9	111.1 (5)
C1—C3—H31	110.1	C7—C8—H81	109.4

C9—C3—H31	110.1	C9—C8—H81	109.4
C1—C3—H32	110.1	C7—C8—H82	109.4
C9—C3—H32	110.1	C9—C8—H82	109.4
H31—C3—H32	108.4	H81—C8—H82	108.0
C1—C4—C5	107.1 (4)	C10—C9—C8	109.5 (5)
C1—C4—H41	110.3	C10—C9—C3	109.3 (4)
C5—C4—H41	110.3	C8—C9—C3	108.4 (4)
C1—C4—H42	110.3	C10—C9—H9	109.9
C5—C4—H42	110.3	C8—C9—H9	109.9
H41—C4—H42	108.5	C3—C9—H9	109.9
C6—C5—C10	110.5 (5)	C9—C10—C5	109.4 (4)
C6—C5—C4	109.7 (5)	C9—C10—H101	109.8
C10—C5—C4	109.4 (4)	C5—C10—H101	109.8
C6—C5—H5	109.1	C9—C10—H102	109.8
C10—C5—H5	109.1	C5—C10—H102	109.8
C4—C5—H5	109.1	H101—C10—H102	108.2

C3—C1—C2—C7	61.4 (5)	C5—C6—C7—C2	−60.8 (6)
C4—C1—C2—C7	−62.9 (5)	C1—C2—C7—C8	−58.8 (5)
Br1—C1—C2—C7	179.5 (3)	C1—C2—C7—C6	60.6 (5)
C4—C1—C3—C9	62.2 (5)	C6—C7—C8—C9	−59.1 (6)
C2—C1—C3—C9	−62.0 (5)	C2—C7—C8—C9	60.7 (5)
Br1—C1—C3—C9	−179.5 (3)	C7—C8—C9—C10	59.1 (5)
C3—C1—C4—C5	−62.2 (5)	C7—C8—C9—C3	−60.0 (5)
C2—C1—C4—C5	62.9 (5)	C1—C3—C9—C10	−60.4 (5)
Br1—C1—C4—C5	179.6 (3)	C1—C3—C9—C8	58.9 (5)
C1—C4—C5—C6	−60.9 (6)	C8—C9—C10—C5	−58.0 (6)
C1—C4—C5—C10	60.5 (5)	C3—C9—C10—C5	60.6 (5)
C10—C5—C6—C7	−60.0 (6)	C6—C5—C10—C9	59.7 (6)
C4—C5—C6—C7	60.7 (6)	C4—C5—C10—C9	−61.2 (5)
C5—C6—C7—C8	59.1 (6)		