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## Structure Reports

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## 1-Bromoadamantane

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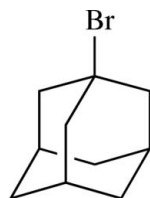
Received 7 November 2008; accepted 18 November 2008

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

The molecule of the title compound,  $\text{C}_{10}\text{H}_{15}\text{Br}$ , 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

 $\text{C}_{10}\text{H}_{15}\text{Br}$ 
 $M_r = 215.13$ 

 Monoclinic,  $P2_1/c$   
 $a = 10.154$  (3) Å  
 $b = 6.8541$  (11) Å  
 $c = 13.240$  (3) Å  
 $\beta = 90.027$  (17)°  
 $V = 921.5$  (4) Å<sup>3</sup>
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 4.40$  mm<sup>-1</sup>  
 $T = 200$  (2) K  
 $0.21 \times 0.16 \times 0.13$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.054$ 

## 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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.38$  e Å<sup>-3</sup>

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

- Chao, M.-H., Kariuki, B. M., Harris, K. D. M., Collins, S. P. & Laundy, D. (2003). *Angew. Chem. Int. Ed.* **42**, 2982–2985.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
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**supplementary materials**

*Acta Cryst.* (2009). E65, o101 [ doi:10.1107/S1600536808038452 ]

## 1-Bromoadamantane

R. Betz, P. Klüfers and P. Mayer

### 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.

### 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.

### 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  $U(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C})$ .

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.

Figures

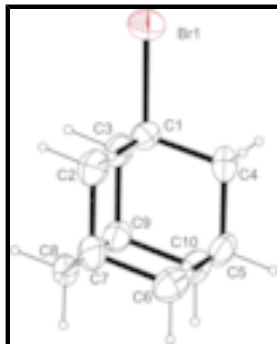


Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

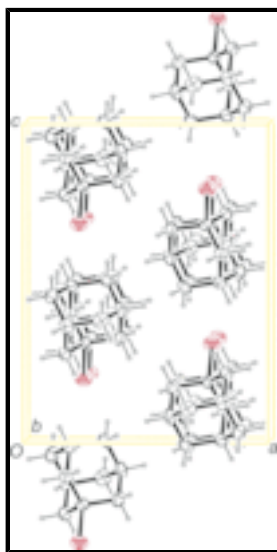


Fig. 2. The packing of the title compound, viewed along [010].

**1-Bromoadamantane**

*Crystal data*

$C_{10}H_{15}Br$

$M_r = 215.13$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 10.154\ (3)\ \text{\AA}$

$b = 6.8541\ (11)\ \text{\AA}$

$c = 13.240\ (3)\ \text{\AA}$

$\beta = 90.027\ (17)^\circ$

$V = 921.5\ (4)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 440$

$D_x = 1.551\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

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

Cell parameters from 2345 reflections

$\theta = 3.9\text{--}26.3^\circ$

$\mu = 4.40\ \text{mm}^{-1}$

$T = 200\ (2)\ \text{K}$

Block, colourless

$0.21 \times 0.16 \times 0.13\ \text{mm}$

*Data collection*

Oxford Xcalibur

1629 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 200(2)$  K

$\omega$  scans

Absorption correction: analytical  
(de Meulenaer & Tompa, 1965)

$T_{\min} = 0.462$ ,  $T_{\max} = 0.614$

4563 measured reflections

1313 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\max} = 25.3^\circ$

$\theta_{\min} = 3.9^\circ$

$h = -12 \rightarrow 11$

$k = -8 \rightarrow 8$

$l = -15 \rightarrow 14$

### 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

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

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

$\Delta\rho_{\max} = 0.77 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|     | <i>x</i>    | <i>y</i>    | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| 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*                           |

## supplementary materials

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|      |            |            |            |             |
|------|------------|------------|------------|-------------|
| 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 ( $\text{\AA}^2$ )

|     | $U^{11}$   | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$    |
|-----|------------|-------------|-------------|--------------|-------------|-------------|
| 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 ( $\text{\AA}$ , $^\circ$ )

|           |           |            |           |
|-----------|-----------|------------|-----------|
| 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)   |               |           |

Fig. 1

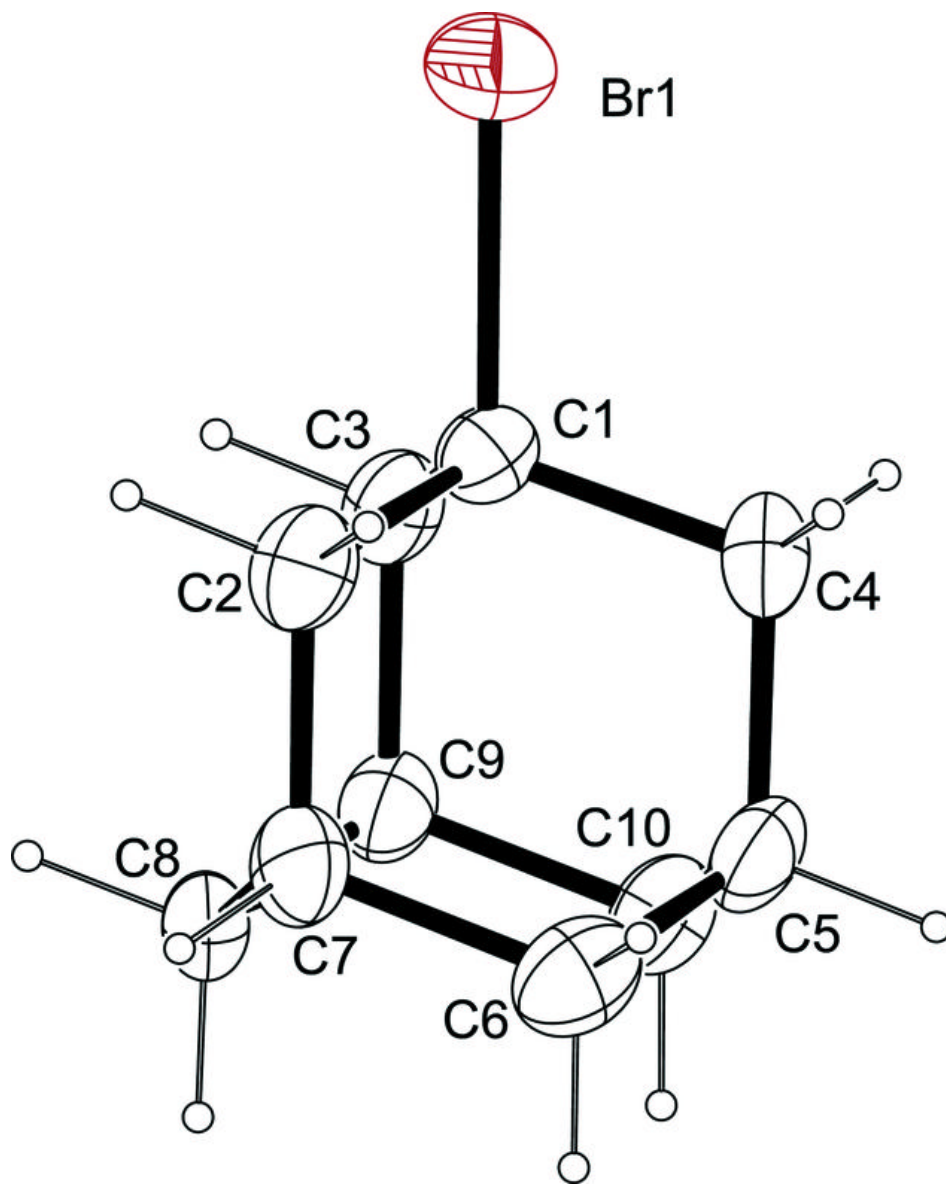


Fig. 2

