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4-Bromobenz[*a*]anthracene

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Abstract. $C_{18}H_{11}Br$, $M_r = 307{\cdot}18$, monoclinic $P2_1/c$, $a = 15{\cdot}93$ (1), $b = 6{\cdot}412$ (6), $c = 25{\cdot}36$ (2) Å, $\beta = 91{\cdot}5$ (1)°, $U = 2589$ Å^3, $Z = 8$, $D_x = 1{\cdot}576$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 45·9 cm^{-1}. Final $R = 0{\cdot}060$ for 1144 observed intensities.

Introduction. As part of a programme of investigations on mono-substituted benz[*a*]anthracenes it was of interest to study the structure of some bromo-substituted derivatives in order to determine whether the substituent causes any appreciable change in the geometry of the aromatic nucleus which is the basis for a great number of cancer-producing substances. The intensities were collected on a Wooster four-circle diffractometer from several crystals mounted about **a** and **b**. There were 1276 independent reflexions with

Table 1. *Atomic positions* (×10^4) *and anisotropic temperature factors* (×10^5) *with e.s.d.'s in parentheses*

Temperature factors are in the form: $T = \exp[-(h^2b_{11} + k^2b_{22} + l^2b_{33} + 2hkb_{12} + 2hlb_{13} + 2klb_{23})]$.

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Molecule I									
Br	1239 (2)	2657 (7)	339 (1)	907 (19)	4558 (139)	157 (5)	502 (53)	−20 (8)	−191 (29)
C(1)	438 (8)	7276 (26)	1666 (5)	409 (68)	1735 (519)	171 (25)	−319 (189)	57 (33)	12 (118)
C(2)	275 (8)	7673 (32)	1114 (6)	366 (73)	3147 (666)	251 (33)	89 (225)	13 (40)	−23 (159)
C(3)	474 (9)	6278 (27)	731 (6)	288 (75)	1931 (569)	230 (32)	303 (172)	−30 (39)	−36 (120)
C(4)	910 (8)	4538 (24)	877 (4)	425 (76)	2380 (557)	57 (19)	−4 (180)	−17 (31)	−69 (77)
C(5)	1510 (9)	2023 (27)	1585 (6)	367 (71)	1787 (687)	172 (26)	14 (185)	−49 (35)	−255 (109)
C(6)	1704 (9)	1627 (25)	2089 (5)	403 (75)	3644 (655)	112 (24)	−178 (165)	18 (34)	−139 (95)
C(7)	1784 (8)	2711 (28)	3018 (5)	294 (64)	2954 (579)	157 (22)	−390 (205)	−112 (31)	9 (133)
C(8)	2015 (9)	3935 (28)	3950 (6)	414 (79)	3933 (650)	142 (27)	−510 (202)	62 (39)	91 (118)
C(9)	1893 (10)	5459 (30)	4332 (6)	524 (93)	2673 (663)	134 (27)	−266 (201)	−16 (41)	100 (112)
C(10)	1490 (10)	7378 (34)	4185 (5)	678 (90)	2883 (676)	125 (24)	−464 (269)	46 (38)	−150 (143)
C(11)	1189 (8)	7710 (27)	3668 (5)	381 (72)	2367 (566)	165 (25)	118 (207)	16 (34)	−446 (120)
C(12)	965 (9)	6539 (22)	2760 (5)	414 (78)	1431 (520)	133 (27)	−318 (151)	4 (36)	−27 (80)
C(13)	883 (8)	5427 (21)	1806 (5)	291 (70)	621 (478)	177 (26)	−350 (149)	−84 (35)	−14 (89)
C(14)	1107 (10)	3988 (26)	1391 (6)	556 (91)	1401 (569)	208 (35)	−198 (191)	−17 (46)	−34 (116)
C(15)	1514 (9)	3139 (24)	2493 (5)	310 (70)	1935 (631)	155 (26)	−233 (171)	47 (34)	26 (71)
C(16)	1100 (7)	5032 (22)	2370 (5)	106 (58)	1506 (492)	141 (23)	43 (145)	44 (29)	11 (90)
C(17)	1273 (8)	6133 (24)	3291 (5)	259 (68)	2040 (552)	154 (26)	−352 (173)	20 (34)	−42 (96)
C(18)	1697 (9)	4202 (26)	3420 (6)	349 (76)	1519 (576)	203 (32)	−173 (183)	39 (40)	267 (110)
Molecule II									
Br	2892 (2)	7455 (6)	645 (1)	711 (17)	3579 (120)	179 (5)	−61 (51)	−71 (7)	−73 (27)
C(1)	4164 (7)	2434 (26)	1749 (5)	326 (62)	1855 (462)	193 (25)	−377 (177)	74 (32)	135 (120)
C(2)	4093 (9)	2705 (28)	1201 (6)	515 (83)	2240 (572)	194 (29)	784 (220)	74 (39)	17 (132)
C(3)	3713 (9)	1224 (27)	881 (5)	350 (74)	2146 (566)	142 (26)	575 (173)	11 (36)	−32 (107)
C(4)	3401 (8)	9426 (22)	1120 (5)	397 (73)	1110 (496)	149 (25)	−324 (150)	26 (34)	75 (85)
C(5)	3132 (9)	7081 (28)	1887 (6)	294 (72)	2528 (684)	264 (37)	432 (194)	−61 (41)	−213 (133)
C(6)	3167 (9)	6787 (22)	2414 (5)	514 (83)	2420 (620)	137 (23)	106 (164)	2 (37)	−281 (89)
C(7)	3504 (8)	8014 (24)	3307 (5)	290 (63)	2951 (619)	110 (22)	−111 (164)	−9 (30)	−57 (99)
C(8)	3778 (9)	9246 (28)	4218 (5)	411 (78)	4381 (677)	128 (26)	614 (194)	52 (38)	92 (110)
C(9)	4086 (9)	767 (28)	4565 (6)	410 (83)	3488 (687)	237 (34)	35 (196)	109 (44)	266 (120)
C(10)	4429 (9)	2672 (31)	4342 (6)	485 (77)	3810 (674)	194 (28)	−157 (229)	42 (37)	396 (147)
C(11)	4453 (9)	3048 (23)	3843 (5)	592 (82)	2376 (606)	143 (24)	−255 (171)	−34 (35)	110 (90)
C(12)	4185 (8)	1786 (22)	2923 (22)	342 (71)	2642 (607)	150 (24)	−8 (150)	−93 (33)	39 (89)
C(13)	3832 (8)	574 (20)	1986 (5)	293 (63)	1192 (463)	129 (22)	579 (144)	73 (32)	−5 (77)
C(14)	3496 (8)	9072 (23)	1656 (5)	334 (73)	1293 (542)	172 (27)	228 (160)	32 (37)	−121 (97)
C(15)	3508 (8)	8398 (20)	2775 (5)	286 (65)	322 (486)	201 (28)	274 (131)	−65 (34)	−16 (83)
C(16)	3840 (7)	295 (20)	2546 (4)	284 (63)	475 (450)	135 (21)	−20 (135)	12 (29)	161 (77)
C(17)	4157 (8)	1446 (23)	3451 (5)	129 (63)	1654 (529)	229 (32)	89 (137)	−16 (36)	−142 (98)
C(18)	3832 (8)	9566 (26)	3654 (6)	287 (71)	2841 (614)	211 (31)	59 (172)	68 (39)	174 (117)

Table 2. *Bond lengths* (Å) *and angles*

	I	II		I	II
Br—C(4)	1·905 (13)	1·912 (14)	C(13)—C(16)	1·48 (2)	1·43 (2)
C(1)—C(2)	1·44 (2)	1·40 (2)	C(15)—C(7)	1·42 (2)	1·37 (2)
C(2)—C(3)	1·36 (2)	1·38 (2)	C(7)—C(18)	1·41 (2)	1·42 (2)
C(3)—C(4)	1·36 (2)	1·40 (2)	C(18)—C(17)	1·44 (2)	1·41 (2)
C(4)—C(14)	1·38 (2)	1·38 (2)	C(17)—C(12)	1·44 (2)	1·36 (2)
C(1)—C(13)	1·42 (2)	1·44 (2)	C(12)—C(16)	1·40 (2)	1·45 (2)
C(13)—C(14)	1·45 (2)	1·38 (2)	C(18)—C(8)	1·43 (2)	1·45 (2)
C(14)—C(5)	1·49 (2)	1·53 (2)	C(8)—C(9)	1·39 (2)	1·39 (2)
C(5)—C(6)	1·33 (1)	1·35 (2)	C(9)—C(10)	1·43 (3)	1·46 (3)
C(6)—C(15)	1·45 (2)	1·47 (2)	C(10)—C(11)	1·40 (2)	1·29 (2)
C(15)—C(16)	1·41 (2)	1·45 (2)	C(11)—C(17)	1·40 (2)	1·49 (2)
C(1)—C(2)—C(3)	123 (2)	121 (2)	C(13)—C(14)—C(5)	114 (1)	120 (1)
C(2)—C(3)—C(4)	118 (1)	118 (1)	C(16)—C(15)—C(7)	120 (1)	124 (1)
C(3)—C(4)—C(14)	125 (1)	122 (1)	C(15)—C(7)—C(18)	121 (1)	118 (1)
C(3)—C(4)—Br	118 (1)	115 (1)	C(7)—C(18)—C(17)	118 (1)	120 (1)
Br—C(4)—C(14)	117 (1)	123 (1)	C(18)—C(17)—C(12)	121 (1)	121 (1)
C(4)—C(14)—C(13)	118 (1)	121 (1)	C(17)—C(12)—C(16)	119 (1)	121 (1)
C(14)—C(13)—C(1)	119 (1)	118 (1)	C(12)—C(16)—C(15)	121 (1)	115 (1)
C(13)—C(1)—C(2)	118 (1)	120 (1)	C(17)—C(18)—C(8)	118 (1)	121 (1)
C(14)—C(5)—C(6)	124 (1)	119 (1)	C(18)—C(8)—C(9)	121 (2)	120 (1)
C(5)—C(6)—C(15)	120 (1)	121 (1)	C(8)—C(9)—C(10)	119 (1)	118 (1)
C(6)—C(15)—C(16)	122 (1)	118 (1)	C(9)—C(10)—C(11)	121 (2)	124 (1)
C(15)—C(16)—C(13)	117 (1)	120 (1)	C(10)—C(11)—C(17)	120 (1)	120 (1)
C(16)—C(13)—C(14)	122 (1)	121 (1)	C(11)—C(17)—C(18)	121 (1)	117 (1)

non-zero intensities, of which 1144 were used in the final refinement.

The structure was determined by the heavy-atom method and refined by full-matrix least squares with anisotropic temperature parameters for Br and C. Scattering factors were those listed in *International Tables for X-ray Crystallography* (1962); the Br scattering factor was corrected for anomalous dispersion. The final R was 0·060 for 1144 observed intensities.*

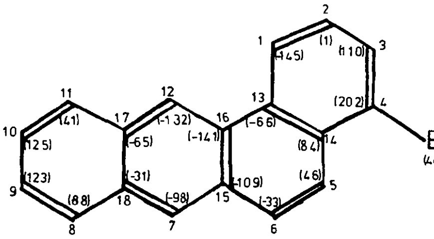
Final parameters are listed in Table 1 and bond lengths and angles in Table 2. Fig. 1 shows the numbering system and the deviations from the mean planes of the two independent molecules in the asymmetric unit. Fig. 2 is a projection of the contents of the unit cell down **b**. The mean planes of molecules I and II are given by $0\cdot89581X+0\cdot40927Y-0\cdot17329Z=1\cdot8487$ and $0\cdot90868X-0\cdot41516Y-0\cdot04411Z=2\cdot3353$ respectively (X is parallel to **a**, Y to **b** and Z is perpendicular to **a** and **b**). Intermolecular contacts $<3\cdot50$ Å are listed in Table 3.

Discussion. The molecules are not as planar as other derivatives of benz[*a*]anthracene and the deviations from the mean planes are different in the two molecules. The Br atom is 0·45 Å out of the plane in I and 0·25 Å in II. This difference is well outside the experi-

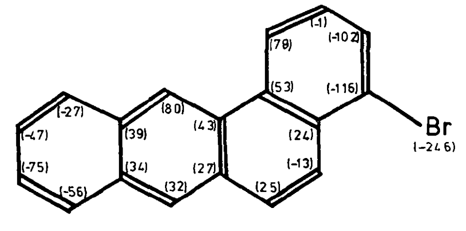
Table 3. *Intermolecular contacts less than* 3·50 Å

C(16)mol. I · · · C(6)mol. II	3·48 (2)
C(1)mol. I · · · C(5)^{i}mol. I	3·50 (2)
C(13)mol. II · · · C(6)^{i}mol. I	3·47 (2)
C(14)mol. II · · · C(6)^{i}mol. I	3·49 (2)
C(1)mol. II · · · C(5)^{i}mol. II	3·43 (2)

Symmetry operation: (i) $x, 1+y, z$.



Molecule I



Molecule II

Fig. 1. The numbering system and deviations (Å × 10^3) of C and Br atoms from the mean planes of the two molecules in the asymmetric unit.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 3198 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

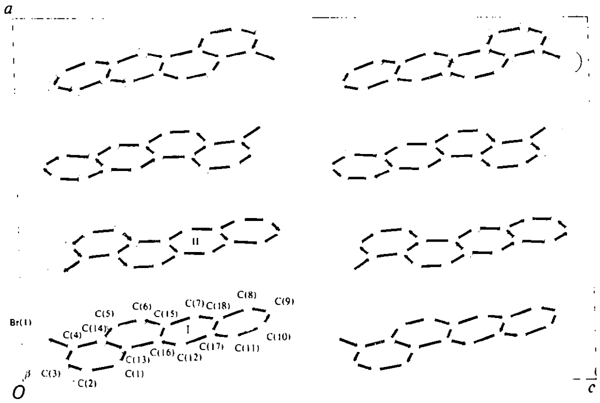

Fig. 2. Contents of the unit cell projected down **b**.

mental error. There is, in each molecule, an angle of 7·2°(I) and 4·8°(II) between the mean plane of the anthracene nucleus and that of the angular ring. In 7,12-dimethylbenz[*a*]anthracene this angle was 18·5° (Iball, 1964). There are large differences between the lengths of corresponding bonds in the two molecules, *e.g.* C(10)–C(11) 1·40, 1·29 Å; C(13)–C(14) 1·45, 1·38 Å; but the bonds in the '*K*' region, C(5)–C(6), are, as expected, short (1·33, 1·35 Å) and in good agreement with the values found in similar compounds, *e.g.* 1,2,5,6-dibenz[*a,h*]anthracene (Iball, Morgan & Zacharias, 1975), 20-methylcholanthrene (Iball & Scrimgeour, 1975) and benzpyrene (Iball, Scrimgeour & Young, 1975). In addition C(13)–C(16) is long in both molecules. Substitution in the angular ring produces non-active compounds and it would seem that it causes more disturbance to the geometry of the parent molecule than would have been expected.

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Cadmium Rubidium Bromide

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Abstract. At room temperature, crystals of $RbCdBr_3$ grown from aqueous solution are isomorphous with $(NH_4)CdCl_3$, *Strukturbericht* type $E2_4$, orthorhombic, space group *Pnma* (D_{2h}^{16}), $a = 9·436$ (4), $b = 4·202$ (2), $c = 15·607$ (3) Å; $Z = 4$, $D_m = 4·68$ (5), $D_x = 4·69$ g cm^{-3}. The structure was determined by X-ray diffraction, $R_2 = 0·058$. Double columns of edge-sharing $CdBr_6$ octahedra (av. Cd–Br = 2·79 Å) extending along **b** are linked by nine-coordinated Rb ions (av. Rb–Br = 3·50 Å) into a compact structure.

Introduction. Precession photographs of colourless $RbCdBr_3$ needles grown from aqueous solution (Natarajan & Secco, 1976) showed orthorhombic symmetry and reflexions only for $hk0$, $h = 2n$; $0kl$, $k + l = 2n$ indicating space groups *Pnma* or $Pn2_1a$. The former space group was assumed and found to give a satisfactory refinement. Accurate lattice parameters were obtained by least-squares fit to the angular settings of 15 reflexions ($19° < 2\theta < 35°$) measured on a Syntax $P\bar{1}$ diffractometer with graphite-crystal monochromated Mo $K\alpha$ radiation ($\lambda = 0·71069$ Å). X-ray intensities of 2101 reflexions in a single quadrant (hkl and $hk\bar{l}$) were measured on the same instrument from a crystal ground into a cylinder of radius 0·075 mm and length (along **b**) 0·3 mm. The intensities were corrected for absorption ($\mu = 32$ mm^{-1}), Lorentz and polarization effects, and symmetry-related reflexions