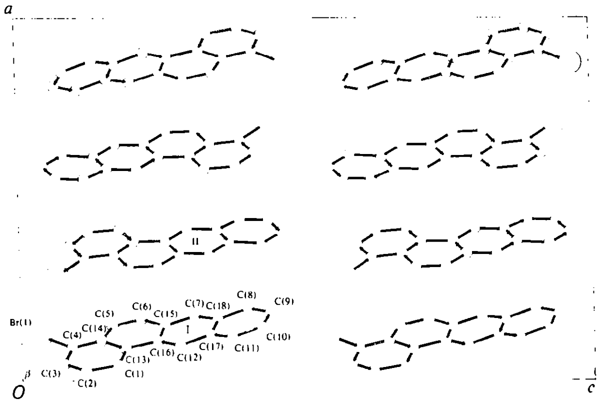

Fig. 2. Contents of the unit cell projected down **b**.

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.

We thank the Cancer Research Campaign and the SRC for financial support. We are grateful to Dr J. Lawrence, Department of Physics, University of St. Andrews and Dr R. Erskine and Mrs E. MacCormick, Computing Centre University of St. Andrews, for their assistance in using the St. Andrews University Computer; also Dr W. D. S. Motherwell, Cambridge, for use of his plotting program *PLUTO*.

References

Iball, J. (1964). *Nature, Lond.* **201**, 916–917.

Iball, J., Morgan, C. H. & Zacharias, D. E. (1975). *J. Chem. Soc. Perkin* II, pp. 1271–1272.

Iball, J. & Scrimgeour, S. N. (1975). *Acta Cryst.* B**31**, 2517–2519.

Iball, J., Scrimgeour, S. N. & Young, D. W. (1975). *Acta Cryst.* B**31**, 328–330.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

Acta Cryst. (1977). B**33**, 127–128

Cadmium Rubidium Bromide

By M. Natarajan Iyer, R. Faggiani and I. D. Brown

Institute for Materials Research,
McMaster University, Hamilton, Ontario, Canada L8S 4M1

(*Received* 10 *May* 1976; *accepted* 25 *June* 1976)

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}), $a = 9\cdot436$ (4), $b = 4\cdot202$ (2), $c = 15\cdot607$ (3) Å; $Z = 4$, $D_m = 4\cdot68$ (5), $D_x = 4\cdot69$ g cm^{-3}. The structure was determined by X-ray diffraction, $R_2 = 0\cdot058$. 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° < 2θ < 35°) measured on a Syntax $P\bar{1}$ diffractometer with graphite-crystal monochromated Mo $K\alpha$ radiation ($\lambda = 0\cdot71069$ 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 correjected for absorption ($\mu = 32$ mm^{-1}), Lorentz and polarization effects, and symmetry-related reflexions were averaged to give 497 unique intensities. The structure was solved from the Patterson diagram and refined by the locally written least-squares program *CUDLS* (CDC 6400) to yield final agreement indices $R_1(=\Sigma\|F_o|-|F_c\|/\Sigma|F_o|) = 0{\cdot}050$ and $R_2\{=[\Sigma\,\omega(F_o-F_c)^2/\Sigma\,\omega F_o^2]^{1/2}\} = 0{\cdot}058$.† In the final refinement $\omega = [\sigma_c^2 + (0{\cdot}01F_o)^2]^{-1}$ where σ_c is the standard error arising from counting statistics, except that $\omega = 0$ for 40 reflexions for which I_o was less than three times its standard error and $|F_c| < |F_o|$. All parameters listed in Table 1 that are not fixed by symmetry were varied together with a scale and an extinction parameter used in the correction $F^* = F[1 + 2{\cdot}8\times10^{-5}\,\beta(2\theta)F^2]^{-1/2}$ (Larson, 1967). The scattering curves for Rb, Cd and Br corrected for anomalous dispersion were taken from *International Tables for X-ray Crystallography* (1962). A final difference electron density map showed no significant features. The bond lengths and angles are given in Table 2.

Discussion. At room temperature, crystals of $RbCdBr_3$ are isostructural with $(NH_4)CdCl_3$ and $RbCdCl_3$ (Brasseur & Pauling, 1938; MacGillavry, Nijveld, Dierdorp & Karsten, 1939). They contain columns of doubled edge-sharing $CdBr_6$ octahedra linked by Rb atoms in tris-monocapped trigonal prismatic coordination. The temperature factors show that all atoms undergo nearly isotropic thermal motions with an r.m.s. amplitude of about 0·18 Å. The structure was checked by a bond-valence analysis* which yielded valence sums around all atoms that showed a standard deviation of only 0·03 valence units from the atomic valence.

The structure is remarkably compact. The density of 4·69 should be compared with 4·27, the mean density of RbBr and $CdBr_2$, and 4·10 g cm^{-3}, the density that would be expected for a perovskite phase that may exist at about 125°C [Natarajan & Secco (1976); see Swanson, McMurdie, Morris & Evans (1967) for a similar transition in $RbCdCl_3$].

We wish to thank the National Research Council of Canada for an operating grant and Dr C. J. L. Lock for helpful discussions.

Table 1. *Atomic positional* (× 10³) *coordinates*

The temperature factor is given by: $\exp(-2\pi^2\sum_i\sum_j U_{ij}H_iH_ja_i^*a_j^*)$. Figures in parentheses are the standard error in the last decimal place quoted.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{13}
Rb	4305 (2)	2500	8260 (1)	36 (1)	27 (1)	30 (1)	–0 (1)
Cd	1651 (2)	2500	564 (1)	31 (1)	30 (1)	28 (1)	–2 (1)
Br(1)	2826 (3)	2500	2089 (1)	29 (1)	31 (1)	24 (1)	–1 (1)
Br(2)	1693 (2)	2500	4950 (1)	25 (1)	21 (1)	26 (1)	–1 (1)
Br(3)	276 (2)	2500	8987 (1)	23 (1)	28 (1)	19 (1)	1 (1)

Table 2. *Interatomic distances* (Å) *and angles* (°)

		Br(3)*	Br(2)*	Br(3)'*
Cd–Br(1)	2·626 (2)	177·4 (5)	94·3 (1)	92·7 (1)
Cd–Br(3)	2·783 (2)		87·6 (1)	85·4 (1)
Cd–Br(2)	2·788 (2)×2		97·8 (1)	172·9 (3), 83·5 (1)
Cd–Br(3)'	2·866 (2)×2			94·3 (1)
Rb–Br(1)	3·435 (2)×2			
Rb–Br(1)	3·470 (3)×2			
Rb–Br(2)	3·501 (2)×2			
Rb–Br(2)	3·589 (2)			
Rb–Br(3)	3·625 (2)			
Rb–Br(3)	3·967 (3)			

* Angles formed between the bond in the left-hand column and the Br atom.

References

BRASSEUR, H. & PAULING, L. (1938). *J. Amer. Chem. Soc.* **60**, 2886–2890.

BROWN, I. D. & SHANNON, R. D. (1973). *Acta Cryst.* A**29**, 266–282.

CRAS, J. A., WILLEMSE, J., GALL, A. W. & HUMMELINK-PETERS, B. G. M. C. (1973). *Rec. Trav. Chim. Pays-Bas*, **92**, 641–650.

International Tables for X-ray Crystallography (1962). Vol. III, pp. 202–216. Birmingham: Kynoch Press.

KETELAAR, J. A. A., RIETDIJK, A. A. & VAN STAVEREN, C. H. (1937). *Rec. Trav. Chim. Pays-Bas*, **56**, 907–908.

LARSON. A. C. (1967). *Acta Cryst.* **23**, 664–665.

MACGILLAVRY, C. H., NIJVELD, H., DIERDORP, S. & KARSTEN, J. (1939). *Rec. Trav. Chim. Pays-Bas*, **58**, 193–200.

NATARAJAN, M. & SECCO, E. A. (1976). *Phys. Stat. Sol.* (*a*), **33**, 427–433.

SWANSON, H. E., MCMURDIE, H. F., MORRIS, M. C. & EVANS, E. H. (1967). Natl. Bur. Stand. Monograph No. 25, Sect. 5, pp. 41–43.

WITTEVEEN, H. T., JONGEJAN, D. L. & BRANDWIJK, V. (1974). *Mater. Res. Bull.* **9**, 345–353.

---

† A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31970 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

* Bond valences (S) were calculated from the bond lengths (R) by the equations: $S=(R/R_0)^{-N}$ where the parameters R_0 and N were fitted to known structures using the method given by Brown & Shannon (1973). The following parameters were determined from the structures listed. Rb–Br: $R_0 = 2{\cdot}605$, $N = 7$ [$RbCdBr_3$, RbBr (2 forms), Rb_2SnBr_6 (Ketelaar, Rietdijk & van Staveren, 1937) and $Rb_2CuCl_2Br_2$ (Witteveen, Jongejan & Brandwijk, 1974)]. Cd–Br: $R_0 = 2{\cdot}307$, $N = 6$ [$RbCdBr_3$, $Cu_3(Bu_2dte)_6.Cd_2Br_6$ (Cras, Willemse, Gall & Hummelink-Peters, 1973)].