The Crystal Structure of $CsIBr_2$

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Summary The anion $(Br–I–Br)^-$ in $CsIBr_2$ is not symmetrical, the longer I–Br bond being 2·78 Å long.

THE crystal structure of $CsIBr_2$ has been investigated to determine the dimensions of the IBr_2^- anion and to compare it with the structures of CsI_3, $CsBr_3$, and CsI_2Br which have been reported previously.[1] These four caesium trihalides are isostructural.[2]

Crystal data: $CsIBr_2$; orthorhombic, space group *Pnma*; $a = 10{\cdot}72 \pm 0{\cdot}02$; $b = 6{\cdot}61 \pm 0{\cdot}02$; $c = 9{\cdot}23 \pm 0{\cdot}02$ Å; $Z = 4$; $D_m = 4{\cdot}29$ g. cm.$^{-3}$,[3] $D_c = 4{\cdot}26$ g. cm.$^{-3}$. All atoms lie on the mirror planes at $y = \frac{1}{4}, \frac{3}{4}$. A total of 243 independent reflections were visually estimated from equi-inclination Weissenberg photographs taken about the *b*-axis with Cu-K_α radiation.

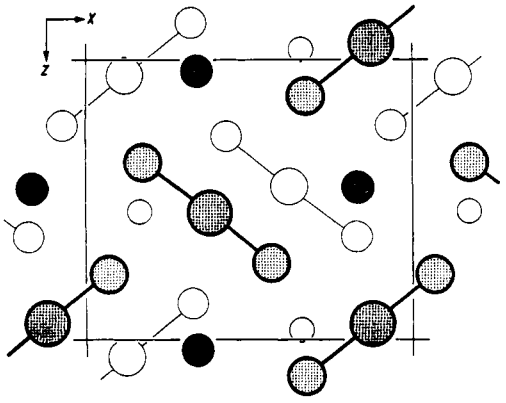

FIGURE. *The structure of* $CsIBr_2$ *projected on to the* ac *plane. The shaded atoms lie at* $y = \frac{1}{4}$, *the outlined ones at* $y = -\frac{1}{4}$ *or* $\frac{3}{4}$. *In order of increasing size the atoms are respectively* Cs, Br, I.

The structure determination was carried out by three-dimensional Fourier methods. Full-matrix least-squares refinement of the structure with individual anisotropic temperature factors has reduced the reliability index to a present value of 0·100 and the final difference synthesis shows no peaks or holes greater than 2 eÅ^{-3}.

The anion is $(Br–I–Br)^-$ and is not symmetrical, which is in accord with the reported geometries of CsI_3 and $CsBr_3$.

Bond lengths and angles in caesium trihalides X(1)–X(2)–X(3)

	X(1)–X(2) Å	X(2)–X(3) Å	∠X(1)–X(2)–X(3)
CsI_3	3·03	2·83	176·0°
$CsBr_3$	2·70	2·44	177·5°
CsI_2Br	2·906	2·777	178·0°
$CsIBr_2$	2·78	2·62	178·0°

The longer I–Br bond (2·78 Å) is considerably shorter than the I–Br bond in CsI_2Br (2·906 Å). Both I–Br bonds are, however, longer than the observed bond length in gaseous IBr (2·485 Å).[4] This would suggest a distortion of the anion due to the other ions within the crystal.[5]

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