Meshueva, 1966). Diese Netze stehen in einem einfachen Zusammenhang mit den ebenen Gitterkomplexen (Smirnova & Poteshnova, 1966). Nichtkubische Kristallstrukturen können durch die Angabe der auftretenden Netze, ihrer Abfolge und Besetzung beschrieben werden (Smirnova, 1967). Wegen dieser wichtigen Anwendungsmöglichkeit möchten wir unsere Literaturzitate durch den Hinweis auf die Arbeiten von Smirnova und Mitarbeiterinnen ergänzen.

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The incoherent X-ray scattering factor of bromine.

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A calculation of the incoherent scattering by bromine has been made by use of the Waller–Hartree formulation including electron exchange and Hartree–Fock–Slater wave functions.

To interpret some results on X-ray solution scattering obtained in this laboratory the incoherent X-ray scattering factor I_{inc} of Br was needed. Following the work of Freeman (see Freeman & Watson, 1962 for references) which shows the great importance of exchange terms in the calculation of I_{inc}, values of I_{inc} were desired based on the Waller–Hartree (1929) formulation. Values of I_{inc} for Br on this basis are not available in the literature; values for all the other halides are available.

The method used for the calculation of the spatially averaged function I_{inc} for an aspherical charge distribution was given by Freeman (1959*a*,*b*) and in his notation I_{inc} for Br is given by

$$
\begin{aligned}
I_{\text{inc}} = 35 - \{ & 2f^2_{1s}(0) + 2f^2_{2s}(0) + 2f^2_{3s}(0) + 2f^2_{4s}(0) \\
& + 6f^2_{2p}(0) + 6f^2_{3p}(0) + 5f^2_{4p}(0) + 10f^2_{3d}(0) \\
& + 12f^2_{2p}(2) + 12f^2_{3p}(2) + 41/5 f^2_{4p}(2) + 100/7 f^2_{3d}(2) \\
& + 1260/49 f^2_{3d}(4) \\
& + 4[f^2_{1s2s}(0) + f^2_{1s3s}(0) + f^2_{1s4s}(0) + f^2_{2s3s}(0) + f^2_{2s4s}(0) + f^2_{3s4s}(0)] \\
& + 12[f^2_{1s2p}(1) + f^2_{2s2p}(1) + f^2_{3s2p}(1) + f^2_{4s2p}(1) + f^2_{1s3p}(1) \\
& + f^2_{2s3p}(1) + f^2_{3s3p}(1) + f^2_{4s3p}(1)] + 10[f^2_{1s4p}(1) + f^2_{2s4p}(1) \\
& + f^2_{3s4p}(1) + f^2_{4s4p}(1)] + 12f^2_{2p3p}(0) + 24f^2_{2p3p}(2) + 10f^2_{2p4p}(0) \\
& + 10f^2_{3p4p}(0) + 20f^2_{2p4p}(2) + 20f^2_{3p4p}(2) \\
& + 20[f^2_{1s3d}(2) + f^2_{2s3d}(2) + f^2_{3s3d}(2) + f^2_{4s3d}(2)] \\
& + 24f^2_{2p3d}(1) + 24f^2_{3p3d}(1) + 36f^2_{2p3d}(3) + 36f^2_{3p3d}(3) \\
& + 20f^2_{4p3d}(1) + 30f^2_{4p3d}(3)\} .
\end{aligned}
$$

Each of the f terms involves an integration of a product of radial wave functions and a spherical Bessel function. In the present work Hartree–Fock–Slater wave functions were used (Herman & Skillman, 1963). The wave functions were available as numerical data and were interpolated to a suitable mesh for computing by the fitting of series of overlapping polynomials of order between 10 and 15. Check calculations were made for $Z = 6$, 7, 13, 14 and were identical with published results (see *International Tables for X-ray Crystallography*, 1962) within 1% for all values of $\sin\theta/\lambda$ provided the same wave functions were used.

The results of the calculations are shown in Table 1. In practice the values would be multiplied by the Breit–Dirac factor.

Table 1. *Incoherent X-ray scattering factor for* Br (*electron units*)

$\sin\theta/\lambda$	I_{inc}	$\sin\theta/\lambda$	I_{inc}
0·00 Å^{-1}	0	0·50 Å^{-1}	14·340
0·01	0·003	0·60	16·241
0·02	0·135	0·70	17·969
0·03	0·299	0·80	19·533
0·04	0·520	0·90	20·938
0·05	0·791	1·00	22·193
0·07	1·451	1·20	24·290
0·10	2·612	1·40	25·916
0·15	4·619	1·60	27·191
0·20	6·481	1·80	28·223
0·30	9·676	2·00	29·082
0·40	12·216		

Note added in proof: – Some calculations of I_{inc}, using Clementi wave functions, which the present results for Br in good agreement, have been found for Z from 1 to 36 (*cf.* Tavard, Nicolas & Roualt, 1967).

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