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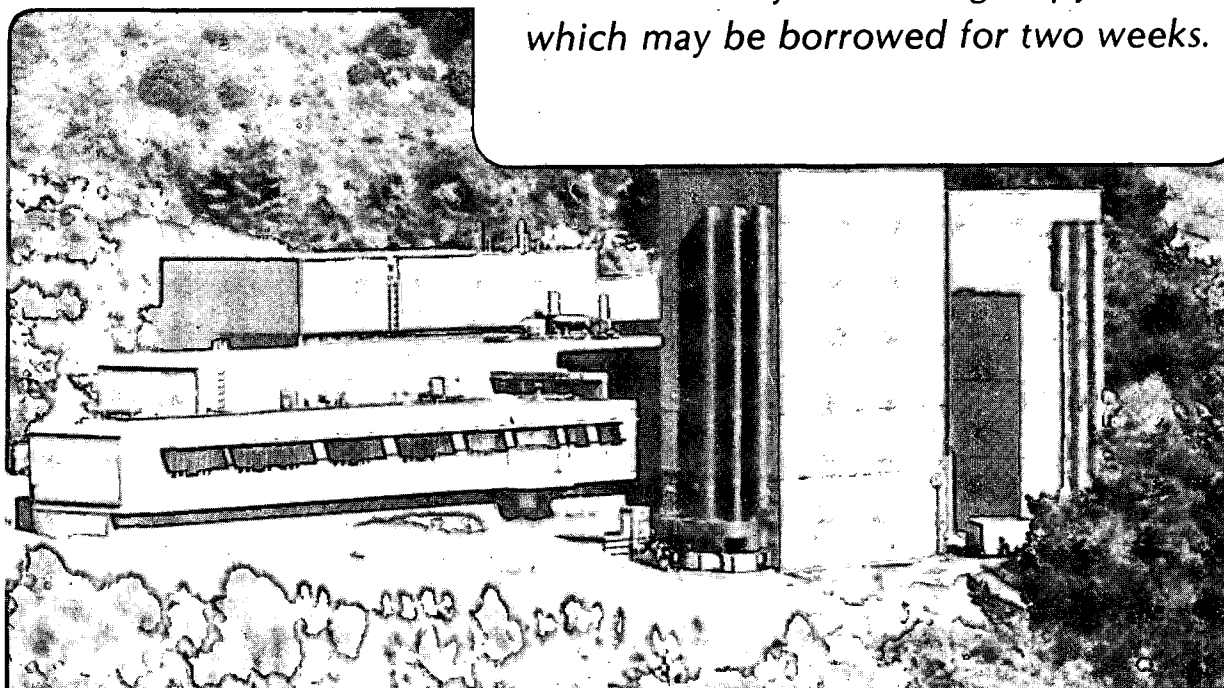
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Relativistic Hartree-Fock X-Ray and Electron Atomic Scattering Factors at High Angles

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Abstract

An enlarged set (atomic number $Z = 2$ to 98) of free atom X-ray atomic scattering (form) factors for high angles ($2\text{Å}^{-1} \leq \sin\theta/\lambda \leq 6\text{Å}^{-1}$) has been calculated based on those of Doyle and Turner [Acta Cryst. A24, 390-397 (1968)]. Four-parameter 'exponential polynomial' fits for these are presented which give far more accurate estimates of the scattering factors at high angles than the Gaussian fits normally used. The use of the Mott formula in conjunction with these new high-angle X-ray form factors allows the calculation of improved accuracy high-angle electron scattering factors. The use of these high accuracy, high-angle scattering factors for important applications such as Fourier charge-density analysis and computer simulation of high resolution electron microscope (HREM) images is discussed.

Introduction

In 1968 Doyle and Turner produced a classic paper tabulating the relativistic Hartree-Fock (RHF) X-ray and electron atomic scattering (form) factors for seventy-six atoms and ions from $\sin\theta/\lambda$ (s) = 0 to 6 Å^{-1}. In addition Doyle and Turner produced nine-parameter Gaussian fits for the X-ray form factors for the angular range s = 0 to 2 Å^{-1} based on the formula

$$f^x(s) = \sum_{i=1}^{4} a_i \exp(-b_i s^2) + c \qquad (1)$$

where the a_i, b_i and c are constants for a given element or ion, and $f^x(s)$ is the X-ray form factor. Subsequently Cromer and Waber (1968) 'filled in the gaps' in Doyle and Turner's

work, and so a complete set of X-ray form factors from Z = 1 to 98 for s = 0 to 2 Å^{-1} with nine parameter Gaussian fits was available. These results are shown in full in International Tables for X-ray Crystallography Volume 4 (1974) and have formed the basis for many computer and other applications requiring X-ray or electron scattering factors. For recent examples see O'Keefe, Buseck and Iijima (1978), Tabbernor, Fox and Fisher (1988) and Peng and Cowley (1988).

However, equation (1) is only applicable to the angular range s = 0 to 2 Å^{-1} and attempts to extend it to higher angles can lead to large errors. For example figure 1(a) shows the Doyle and Turner Gaussian fit to the calculated f^x(s) for nitrogen (Z = 7) extrapolated to s = 6 Å^{-1}; it can be seen that the curve based on equation (1) drops well below the true values calculated by Doyle and Turner (1968), and in fact goes negative for s > 3 Å^{-1}. Another example, uranium (Z= 92), is shown in figure 1(b), and in this case the extrapolated Gaussian values are far too high. It is clear from this discussion that an accurate set of high-angle form factors for all elements from s = 2 Å^{-1} to 6 Å^{-1} is necessary, and that a n-parameter curve fitting routine for this angular range is highly desirable; this is the object of the present work.

Calculations

(1) High-Angle Form Factors-- As mentioned previously, Doyle and Turner (1968) calculated form factors for seventy-six atoms and ions up to s = 6 Å^{-1}. The elements they omitted to consider were those with atomic number, Z = 1, 39 - 41, 43 - 46, 52, 57 - 62, 64 - 79, 81, 84 - 85, 87 - 91 and 93 - 98. It is therefore necessary to calculate the high-angle form factors for all these elements; this could be done from first principles in the manner of Doyle and Turner or Cromer and Waber (1968). This, however, is very time consuming and tedious, and in this work a simpler alternative is discussed.

For hydrogen at angles for which s ≥ 1.5 Å^{-1}, the X-ray form factor is less than 2 × 10^{-3} (see for example Stewart, Davidson and Simpson, 1965) and can therefore be considered to be virtually zero for these high angles.

For elements in the range Z = 35 - 92, the variation of f^x with Z for the Doyle and Turner (1968) values was investigated, and it was found that they fell on a slowly varying smooth curve which is very close to linear for high Z. A simple polynomial curve-fitting routine available in the Cricket Graph ^{TM} software for an Apple - McIntosh personal computer was used to fit the f^x versus Z data for the appropriate values of s in order to 'fill in the gaps' in Doyle and Turner's values, and a correlation coefficient of 0.999 or better was obtained in each case with appropriate choice of polynomial coefficients; an example for s = 3 $Å^{-1}$ is shown in figure 2. Interpolation using these curve fits allowed the evaluation of the high-angle X-ray form factors for the atomic numbers not considered by Doyle and Turner up to Z = 91.

For the elements with Z = 93 - 98, a simple linear extrapolation from the f^x versus Z variation (Z = 63 - 92) of the values of Doyle and Turner (1968) for 2 $Å^{-1}$ ≤ s ≤ 6 $Å^{-1}$ was used. This is likely to be a little less accurate than the interpolative method described previously, but still good (and certainly much better than the Gaussian fits) as the form of f^x versus Z is close to linear in the range Z = 63 - 92, as shown in figure 3 for s = 3 $Å^{-1}$.

The foregoing calculations together with the values of Doyle and Turner (1968) allowed a tabulation of the X-ray form factors for s = 2.5, 3.0, 3.5, 4.0, 5.0, 6.0 $Å^{-1}$ for all elements (Z = 2 - 98) and these are shown in table 1. It is also satisfactory to use these for ions, as the ionic form factors of Cromer and Waber (1968) and Doyle and Turner for 2 $Å^{-1}$ are very close to the free atom values; this is of course not surprising, as ionicity only significantly affects low-angle scattering factors which reflect the behaviour of valence electrons.

(2) Parametric Curve-Fitting Routines--Initially an attempt was made to fit accurately the full range of $f^x(s)$ values for s = 0 to 6 $Å^{-1}$. It soon became apparent that this would be an impossible task with any conventional curve fitting routines such as polynomial or Gaussian, and so to obtain accurate high-angle form factors for arbitrary values of s in the range 2$Å^{-1}$ ≤ s ≤ 6$Å^{-1}$ the values of table 1 only were considered. A simple, yet seemingly

quite reasonable approach to the fit is linear interpolation between the values shown in table 1, although it is difficult to estimate the errors at the mid-way points between the tabulated values. For computer applications it is more convenient to have a n-parameter function to fit the $f^x(s)$ versus s variation, and initially a conventional Tchebyshev polynomial curve fit was tried; it soon became clear from the shape of the $f^x(s)$ versus s curves for $2 \text{ Å}^{-1} \leq s \leq 6 \text{ Å}^{-1}$ that an exponential or logarithmic expression would provide a better fit. Accordingly, expressions of the form

$$f^x(s) = a \, s^{-b} \qquad (2a)$$

$$\text{and} \quad f^x(s) = a \exp(-bs) \qquad (2b)$$

(where a and b are constants which depend on atomic number, Z) were fitted using the Cricket Graph™ software on the Apple McIntosh personal computer. This resulted in an improvement over the polynomial fits, but the correlation coefficients, R, for these fits could still drop below 0.99. For example, for equation (2a) for silicon (Z=14), a = 3.7856, b = 1.4668 and R = 0.976 which gave errors of up to 13% in the interpolated values of $f^x(s)$.

In order to improve the accuracy of fit, a three parameter polynomial fit based on equation (2b) in the following form was tried

$$\ln[f^x(s)] = a_0 + a_1 s + a_2 s^2 \qquad (3)$$

This expression resulted in a minimum R value of 0.993 at Z = 22, corresponding to a maximum error of 8.8% in $f^x(s)$ at $s = 2.5 \text{Å}^{-1}$ for titanium.

To improve matters still further a four-parameter fit of the form

$$\ln[f^x(s)] = a_0 + a_1 s + a_2 s^2 + a_3 s^3 \qquad (4)$$

was adopted and the correlation coefficient R remained at 0.999 or above, except for Z = 95 - 97 where it dropped to 0.9985 and for Z = 98 for which R was found to be 0.998. The values of a_0, a_1, a_2, a_3 and R for all Z derived in this way from equation (4) are shown in table 2. This use of equation (4) resulted in a maximum error in $f^x(s)$ of 5.0% which occurred for californium (Z = 98) at $s = 2.5 \text{Å}^{-1}$. For most other elements the maximum

errors in $f^x(s)$ are below 3%, which is much better than the errors given by the Gaussian fits. As discussed by Doyle and Turner (1968) the percentage error in $f^x(s)$ is perhaps better expressed as a function of $f^x(0)$. For $Z = 98$ at $s = 2.5\text{Å}^{-1}$ we find that $\partial f^x(s)/f^x(0) \times 100$ (where $\partial f^x(s)$ is the error on $f^x(s)$) is equal to 0.008; this error is about the same as the best equivalent average error values quoted by Doyle and Turner for their Gaussian fits in the range $s = 0$ to 2Å^{-1}. All other fitted values of the present work give values of $\partial f^x(s)/f^x(0) \times 100$ smaller than 0.008.

To check the accuracy of the curve fitting on the personal computer, equation (4) was used to fit the $\ln[f^x(s)]$ versus s data on a mainframe computer with polynomial curve-fitting NAG routines E02ADF and E02AEF, and the interpolated values of $f^x(s)$ obtained using the NAG routines agreed to within 1 part in 10^4 with those generated by the personal computer.

Electron Scattering Factors

The electron scattering factor, $f^e(s)$, is related to the X-ray scattering factor by the usual Mott formula

$$f^e(s) = \frac{me^2}{2h^2}\left(\frac{\lambda}{\sin\theta}\right)^2\left(Z - f^x(s)\right) \tag{5}$$

which reduces to

$$f^e(s) = 0.023934\left(\frac{1}{s}\right)^2\left(Z - f^x(s)\right) \tag{6}$$

where $f^e(s)$ is a scattering length expressed in Å. Hence a complete set of high angle electron scattering factors can be obtained by the use of equation (6) and table 2 except for hydrogen where the simple use of equation (6) with $f^x = 0$ is very satisfactory. If ∂f^x is the error on f^x and ∂f^e the error on f^e, then differentiating (6) gives

$$\frac{\partial f^e}{f^e} = \frac{\partial f^x}{Z - f^x} \tag{7}$$

which means that the larger s, the smaller f^x and the smaller the error in f^e. For higher angles f^x is smaller, and so the error in f^e is even smaller. As for f^x, the greatest error in f^e

occurred for Z = 98 at s = 2.5Å⁻¹ and was 0.93%. All errors in f^e calculated by this method are therefore less than 1.0%, which is more than adequate for most applications.

It is worth noting that the use of the nine-parameter Gaussian fitted X-ray form factors of Doyle and Turner (1968) for 0Å⁻¹ ≤ s ≤ 2Å⁻¹ and the four-parameter fits of the present work for 2Å⁻¹ ≤ s ≤ 6Å⁻¹ together with the Mott formula generally gives better interpolated electron scattering factor values than the eight-parameter Gaussian fit for f^e(s) quoted by Doyle and Turner. This is true except for very low angles (s ≤ 0.04Å⁻¹) when Z - f^x is small, and in this case the procedure adopted by O'Keefe et al.(1978) and described in detail by Peng and Cowley (1988) should be used so that large errors in f^e are avoided for small s.

Examples of applications for high-angle form factors

(1) Electron charge-density calculations--These are important for determining the distribution of electrons around atoms in crystalline solids. The electron charge density, ρ (x,y,z), at position vector **r** (x,y,z) in a unit cell is given by

$$\rho\ (x,y,z) = \frac{1}{\Omega}\sum_h \sum_k \sum_l F_{hkl} \exp\ [-2\pi i\ (hx + ky + lz)] \tag{8}$$

where Ω is the volume of the unit cell and F_{hkl} are the X-ray structure factors for planes with Miller indices (hkl). For copper, Smart and Humphreys (1978) have shown that for the Fourier series of equation (8) to converge, well over 1200 terms are needed. This has been confirmed by Tabbernor (1988) who also found that similar numbers of structure factors are needed for convergence of the charge density series of other elements. This means that many high angle structure factors which occur in the range 2 Å⁻¹ ≤ s ≤ 6Å⁻¹ are needed for such calculations, and this is an important application for the high-angle form factors presented here.

<u>(2) Simulation of HREM images</u>--The dynamical electron scattering calculation for the simulation of high resolution electron microscope images requires a numerical evaluation of the crystal potential. This evaluation is normally carried out by Fourier transformation of the structure factors (for electrons), F_{hkl}, for the structure being simulated. In the case of the commonly used 'multislice' dynamical scattering algorithm (Goodman and Moodie, 1974), the structure factor calculation requires accurately-known scattering factors out to twice the scattering angle of the highest-order diffracted beam included in the computation (O'Keefe and Kilaas, 1988). In order to maintain sufficient precision, diffracted beams out to values of h,k,l corresponding to reciprocal lattice vectors of 3 or 4 reciprocal Ångstroms should be included in the computation; thus scattering factors are required for values out to $s = 3$ or 4 Å^{-1}, equivalent to lattice vectors of 6 to 8 Å^{-1}. Computations for structures that include heavy atoms, or for higher voltage microscopes, increase the requirement for form factors accurate at higher angles, due to the heavier scattering and flatter Ewald spheres involved.

For image simulations, it is convenient to be able store scattering factors in the form of parameterised fits to the scattering curves. Lack of suitable complete tables of parameterised fits of electron form factors has led to the widespread use of the Gaussian fits of the International Tables for Crystallography for the X-ray form factors followed by conversion to the electron values by the Mott formula (equation 5). As discussed previously this can lead to very poor accuracy form factors for $s \geq 2$ Å^{-1} and the procedures recomended in the present work improve matters considerably.

Summary and Conclusions

The effect of extending the Gaussian fits for X-ray form factors, f^x, presented in the International Tables for X-ray Crystallography(1974) to high angles (2 Å$^{-1} \leq s \leq 6$ Å^{-1}) has been carefully investigated, and it has been found that errors as high as a hundred percent in f^x can occur, and that in some cases f^x can even go negative (see for example figure 1a for nitrogen) if this approach is adopted. For the electron scattering factors, f^e, derived

by the Mott formula from these high-angle X-ray form factors, the situation is not as catastrophic, but errors in f^e as high as ten per-cent can often be encountered.

It is clear that such inaccuracies are not acceptable when performing the Fourier analyses necessary for charge density studies or HREM image simulations, and in the present work an alternative method of producing high-angle X-ray and electron form factors is discussed. This has involved curve fitting the f^x versus Z variation of the RHF values of Doyle and Turner (1968), so that a complete set of form factors from 2 - 6 Å^{-1} is available for all elements from Z = 1 through 98. From these form factors, a four-parameter 'exponential polynomial' curve fitting of the variation of f^x with s has been made. Accurate values of the electron scattering factors were then calculated with the Mott formula in the usual way.

This procedure would appear to generate a maximum error of only about 5.0% in the X-ray scattering factors (for Z = 98 (californium) with s = 2.5 Å^{-1}) which is far more satisfactory than the Gaussian approach. If these best X-ray form factors are converted to electron scattering factors, by the Mott formula the maximum error encountered in f^e is less than 1.0% which is more than adequate for most applications.

Acknowledgements

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Table 1 High-angle X-ray atomic scattering factors

s	2.0	2.5	3.0	3.5	4.0	5.0	6.0
He	0.010	0.004	0.002	0.001	0.001	0.000	0.000
Li	0.044	0.021	0.011	0.006	0.004	0.002	0.001
Be	0.120	0.060	0.033	0.019	0.012	0.005	0.003
B	0.233	0.126	0.072	0.043	0.027	0.012	0.006
C	0.373	0.216	0.130	0.081	0.053	0.025	0.013
N	0.525	0.324	0.204	0.132	0.088	0.043	0.023
O	0.674	0.443	0.292	0.196	0.134	0.067	0.037
F	0.810	0.564	0.389	0.270	0.190	0.099	0.055
Ne	0.929	0.680	0.489	0.331	0.254	0.137	0.079
Na	1.032	0.791	0.591	0.438	0.325	0.183	0.107
Mg	1.120	0.892	0.691	0.527	0.401	0.234	0.141
Al	1.195	0.979	0.783	0.615	0.478	0.290	0.179
Si	1.264	1.056	0.867	0.699	0.556	0.349	0.222
P	1.333	1.122	0.942	0.777	0.632	0.411	0.268
S	1.411	1.182	1.009	0.849	0.705	0.474	0.316
Cl	1.502	1.240	1.069	0.915	0.773	0.536	0.367
Ar	1.614	1.301	1.123	0.974	0.836	0.597	0.419
K	1.748	1.367	1.174	1.028	0.895	0.657	0.472
Ca	1.908	1.444	1.225	1.078	0.949	0.715	0.524
Sc	2.090	1.533	1.279	1.125	0.998	0.770	0.577
Ti	2.290	1.637	1.338	1.171	1.044	0.821	0.627
V	2.506	1.756	1.404	1.217	1.087	0.869	0.677
Cr	2.727	1.888	1.479	1.266	1.129	0.914	0.724
Mn	2.963	2.037	1.563	1.319	1.171	0.956	0.769
Fe	3.195	2.197	1.658	1.377	1.213	0.995	0.813
Co	3.424	2.366	1.763	1.441	1.258	1.033	0.853
Ni	3.647	2.543	1.878	1.512	1.306	1.069	0.892
Cu	3.855	2.721	2.001	1.590	1.358	1.105	0.929
Zn	4.063	2.908	2.135	1.677	1.414	1.140	0.964
Ga	4.260	3.097	2.277	1.772	1.477	1.176	0.998
Ge	4.447	3.287	2.428	1.876	1.545	1.213	1.030
As	4.621	3.475	2.584	1.988	1.621	1.251	1.061
Se	4.782	3.658	2.745	2.108	1.703	1.292	1.092
Br	4.932	3.836	2.909	2.235	1.793	1.337	1.123
Kr	5.071	4.007	3.074	2.369	1.890	1.384	1.154
Rb	5.200	4.168	3.239	2.507	1.993	1.436	1.186
Sr	5.323	4.320	3.401	2.649	2.103	1.493	1.219
Y	5.440	4.460	3.560	2.780	2.215	1.550	1.250
Zr	5.558	4.590	3.720	2.920	2.335	1.620	1.285
Nb	5.680	4.710	3.860	3.065	2.405	1.690	1.327
Mo	5.813	4.827	3.988	3.217	2.581	1.766	1.373
Tc	5.946	4.930	4.110	3.350	2.690	1.840	1.420
Ru	6.097	5.040	4.230	3.485	2.820	1.925	1.470
Rh	6.262	5.140	4.350	3.620	2.940	2.012	1.520
Pd	6.443	5.240	4.460	3.740	3.080	2.100	1.575
Ag	6.651	5.351	4.566	3.862	3.207	2.206	1.635
Cd	6.871	5.461	4.665	3.977	3.330	2.304	1.698
In	7.110	5.577	4.761	4.087	3.449	2.406	1.746
Sn	7.367	5.702	4.853	4.192	3.565	2.509	1.835

Table 1 (continued)

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s	2.0	2.5	3.0	3.5	4.0	5.0	6.0
Sb	7.642	5.836	4.945	4.292	3.678	2.615	1.909
Te	7.921	5.980	5.040	4.390	3.780	2.722	1.990
I	8.239	6.142	5.132	4.478	3.891	2.828	2.067
Xe	8.556	6.315	5.229	4.566	3.991	2.935	2.150
Cs	8.881	6.502	5.332	4.651	4.087	3.041	2.237
Ba	9.213	6.704	5.440	4.735	4.178	3.146	2.325
La	9.550	6.917	5.550	4.820	4.270	3.240	2.410
Ce	9.858	7.117	5.663	4.910	4.360	3.340	2.490
Pr	10.166	7.333	5.800	5.000	4.445	3.435	2.580
Nd	10.473	7.567	5.930	5.090	4.525	3.530	2.670
Pm	10.773	7.817	6.088	5.180	4.600	3.625	2.770
Sm	11.064	8.083	6.250	5.280	4.675	3.720	2.865
Eu	11.345	8.348	6.435	5.378	4.750	3.812	2.965
Gd	11.631	8.683	6.588	5.490	4.830	3.905	3.070
Tb	11.886	8.983	6.775	5.610	4.915	3.990	3.170
Dy	12.141	9.267	6.963	5.720	5.000	4.075	3.270
Ho	12.392	9.533	7.163	5.850	5.090	4.155	3.355
Er	12.621	9.783	7.375	5.980	5.180	4.235	3.440
Tm	12.847	10.033	7.588	6.110	5.280	4.310	3.520
Yb	13.064	10.267	7.788	6.250	5.380	4.380	3.600
Lu	13.277	10.500	8.013	6.400	5.490	4.450	3.680
Hf	13.481	10.733	8.238	6.560	5.600	4.520	3.755
Ta	13.679	10.950	8.480	6.740	5.710	4.585	3.825
W	13.871	11.167	8.706	6.900	5.840	4.650	3.900
Re	14.057	11.383	8.938	7.080	5.960	4.715	3.970
Os	14.239	11.583	9.163	7.270	6.080	4.788	4.035
Ir	14.418	11.783	9.400	7.460	6.210	4.860	4.105
Pt	14.595	11.983	9.620	7.650	6.340	4.935	4.175
Au	14.770	12.168	9.826	7.878	6.489	5.010	4.244
Hg	14.949	12.360	10.049	8.081	6.644	5.090	4.310
Tl	15.131	12.530	10.270	8.290	6.800	5.175	4.374
Pb	15.317	12.724	10.482	8.495	6.973	5.260	4.441
Bi	15.510	12.896	10.690	8.704	7.145	5.351	4.505
Po	15.711	13.060	10.900	8.910	7.320	5.440	4.567
At	15.922	13.230	11.090	9.120	7.500	5.540	4.630
Rn	16.143	13.386	11.282	9.329	7.686	5.650	4.702
Fr	16.377	13.550	11.460	9.530	7.878	5.755	4.768
Ra	16.623	13.700	11.640	9.730	8.070	5.870	4.840
Ac	16.880	13.860	11.815	9.930	8.255	5.933	4.910
Th	17.149	14.020	11.980	10.130	8.440	6.118	4.982
ⁱPa	17.423	14.180	12.150	10.320	8.630	6.250	5.055
U	17.713	14.341	12.294	10.495	8.823	6.378	5.136
Np	18.012	14.503	12.475	10.695	9.008	6.489	5.206
Pu	18.319	14.664	12.656	10.895	9.193	6.602	5.275
Am	18.640	14.826	12.838	11.095	9.378	6.713	5.345
Cm	18.975	14.988	13.019	11.295	9.563	6.825	5.414
Bk	19.315	15.150	13.200	11.495	9.748	6.937	5.484
Cf	19.665	15.311	13.381	11.695	9.933	7.049	5.553

Table 2: Parameters for the fit of ln[f^x(s)] in equation (4)

Z	Symbol	a0	a1	a2 (x10)	a3 (x100)	R factor
2	He	0.52543	-3.43300	4.80070	-2.54760	1.0000
3	Li	0.89463	-2.43660	2.32500	-0.71949	1.0000
4	Be	1.25840	-1.94590	1.30460	-0.04297	1.0000
5	B	1.66720	-1.85560	1.60440	-0.65981	1.0000
6	C	1.70560	-1.56760	1.18930	-0.42715	1.0000
7	N	1.54940	-1.20190	0.51064	0.02472	1.0000
8	O	1.30530	-0.83742	-0.16738	0.47500	1.0000
9	F	1.16710	-0.63203	-0.40207	0.54352	1.0000
10	Ne	1.09310	-0.50221	-0.53648	0.60957	0.9995
11	Na	0.84558	-0.26294	-0.87884	0.76974	1.0000
12	Mg	0.71877	-0.13144	-1.20900	0.82738	1.0000
13	Al	0.67975	-0.08756	-0.95431	0.72294	1.0000
14	Si	0.70683	-0.09888	-0.98356	0.55631	1.0000
15	P	0.85532	-0.21262	-0.37390	0.20731	1.0000
16	S	1.10400	-0.40325	0.20094	-0.26058	1.0000
17	Cl	1.42320	-0.63936	0.84722	-0.76135	0.9995
18	Ar	1.82020	-0.92776	1.59220	-1.32510	0.9995
19	K	2.26550	-1.24530	2.38330	-1.91290	0.9990
20	Ca	2.71740	-1.55670	3.13170	-2.45670	0.9990
21	Sc	3.11730	-1.81380	3.71390	-2.85330	0.9990
22	Ti	3.45360	-2.01150	4.13170	-3.11710	0.9995
23	V	3.71270	-2.13920	4.35610	-3.22040	0.9995
24	Cr	3.87870	-2.19000	4.38670	-3.17520	1.0000
25	Mn	3.98550	-2.18850	4.27960	-3.02150	1.0000
26	Fe	3.99790	-2.11080	3.98170	-2.71990	1.0000
27	Co	3.95900	-1.99650	3.60630	-2.37050	1.0000
28	Ni	3.86070	-1.88690	3.12390	-1.94290	1.0000
29	Cu	3.72510	-1.65500	2.60290	-1.49760	0.9995
30	Zn	3.55950	-1.45100	2.03390	-1.02160	0.9995
31	Ga	3.37560	-1.23910	1.46160	-0.55471	0.9995
32	Ge	3.17800	-1.02230	0.89119	-0.09984	0.9995
33	As	2.97740	-0.81038	0.34861	0.32231	0.9995
34	Se	2.78340	-0.61110	-0.14731	0.69837	0.9995
35	Br	2.60610	-0.43308	-0.57381	1.00950	0.9995
36	Kr	2.44280	-0.27244	-0.95570	1.27070	0.9995
37	Rb	2.30990	-0.14328	-1.22600	1.45320	1.0000
38	Sr	2.21070	-0.04770	-1.41100	1.55410	1.0000
39	Y	2.14220	0.01935	-1.52240	1.59630	1.0000
40	Zr	2.12690	0.08618	-1.49190	1.51820	1.0000
41	Nb	2.12120	0.05381	-1.50070	1.50150	1.0000
42	Mo	2.18870	-0.00655	-1.25340	1.24010	1.0000
43	Tc	2.25730	-0.05737	-1.07450	1.06630	1.0000
44	Ru	2.37300	-0.15040	-0.77694	0.79060	0.9995
45	Rh	2.50990	-0.25906	-0.44719	0.49443	0.9995
46	Pd	2.67520	-0.39137	-0.05894	0.15404	0.9995
47	Ag	2.88690	-0.56119	0.42189	-0.25659	0.9990
48	Cd	3.08430	-0.71450	0.84482	-0.60990	0.9990
49	In	3.31400	-0.89697	1.35030	-1.03910	0.9990
50	Sn	3.49840	-1.02990	1.68990	-1.29860	0.9990

Table 2: Parameters for the fit of ln[f^x(s)] (continued).

Z	Symbol	a0	a1	a2 (x10)	a3 (x100)	R factor
51	Sb	3.70410	-1.18270	2.08920	-1.61640	0.9990
52	Te	3.88240	-1.30980	2.41170	-1.86420	0.9990
53	I	4.08010	-1.45080	2.76730	-2.13920	0.9990
54	Xe	4.24610	-1.56330	3.04200	-2.34290	0.9990
55	Cs	4.38910	-1.65420	3.25450	-2.49220	0.9995
56	Ba	4.51070	-1.72570	3.41320	-2.59590	0.9995
57	La	4.60250	-1.77070	3.49970	-2.64050	0.9995
58	Ce	4.68890	-1.81690	3.60090	-2.70550	0.9995
59	Pr	4.72150	-1.81390	3.56480	-2.65180	0.9995
60	Nd	4.75090	-1.80800	3.51970	-2.59010	1.0000
61	Pm	4.74070	-1.76600	3.37430	-2.44210	1.0000
62	Sm	4.71700	-1.71410	3.20800	-2.28170	1.0000
63	Eu	4.66940	-1.64140	2.98580	-2.07460	1.0000
64	Gd	4.61010	-1.55750	2.73190	-1.84040	0.9995
65	Tb	4.52550	-1.45520	2.43770	-1.57950	0.9995
66	Dy	4.45230	-1.36440	2.17540	-1.34550	0.9990
67	Ho	4.37660	-1.27460	1.92540	-1.13090	0.9990
68	Er	4.29460	-1.18170	1.67060	-0.91467	0.9990
69	Tm	4.21330	-1.09060	1.42390	-0.70804	0.9990
70	Yb	4.13430	-1.00310	1.18810	-0.51120	0.9990
71	Lu	4.04230	-0.90518	0.92889	-0.29820	0.9990
72	Hf	3.95160	-0.80978	0.67951	-0.09620	0.9990
73	Ta	3.85000	-0.70599	0.41103	0.11842	0.9990
74	W	3.76510	-0.61807	0.18568	0.29787	0.9990
75	Re	3.67600	-0.52688	-0.04706	0.48180	0.9995
76	Os	3.60530	-0.45420	-0.22529	0.61700	0.9995
77	Ir	3.53130	-0.37856	-0.41174	0.75967	0.9995
78	Pt	3.47070	-0.31534	-0.56487	0.87492	0.9995
79	Au	3.41630	-0.25987	-0.69030	0.96224	0.9995
80	Hg	3.37350	-0.21428	-0.79013	1.02850	1.0000
81	Tl	3.34590	-0.18322	-0.84911	1.05970	1.0000
82	Pb	3.32330	-0.15596	-0.89878	1.08380	1.0000
83	Bi	3.31880	-0.14554	-0.90198	1.06850	1.0000
84	Po	3.32030	-0.13999	-0.89333	1.04380	1.0000
85	At	3.34250	-0.15317	-0.83350	0.97641	1.0000
86	Rn	3.37780	-0.17800	-0.74320	0.88510	1.0000
87	Fr	3.41990	-0.20823	-0.64000	0.78354	0.9995
88	Ra	3.47530	-0.25005	-0.50660	0.65836	0.9995
89	Ac	3.49020	-0.25109	-0.49651	0.64340	0.9995
90	Th	3.61060	-0.35409	-0.18926	0.36849	0.9995
91	Pa	3.68630	-0.41329	-0.01192	0.20878	0.9995
92	U	3.76650	-0.47542	0.16850	0.05060	0.9990
93	Np	3.82870	-0.51955	0.29804	-0.06566	0.9990
94	Pu	3.88970	-0.56296	0.42597	-0.18080	0.9990
95	Am	3.95060	-0.60554	0.54967	-0.29112	0.9985
96	Cm	4.01470	-0.65062	0.67922	-0.40588	0.9985
97	Bk	4.07780	-0.69476	0.80547	-0.51729	0.9985
98	Cf	4.14210	-0.73977	0.93342	-0.62981	0.9980

Figure Legends

Figure 1a Graph of X-ray scattering factor, f^x, versus $\sin\theta/\lambda$ for nitrogen (Z=7) showing the Gaussian fit going negative at high angles.

Figure 1b Graph of f^x versus $\sin\theta/\lambda$ for uranium (Z=92) showing the Gaussian fit to be too high for high angles.

Figure 2 Graph of X-ray scattering factor, f^x, versus atomic number, Z, for $\sin\theta/\lambda = 3$ Å^{-1} showing the polynomial fit to the values of Doyle and Turner (1968).

Figure 3 As figure 2 but showing the linear variation of f^x with atomic number Z = 63 to 92.

URANIUM
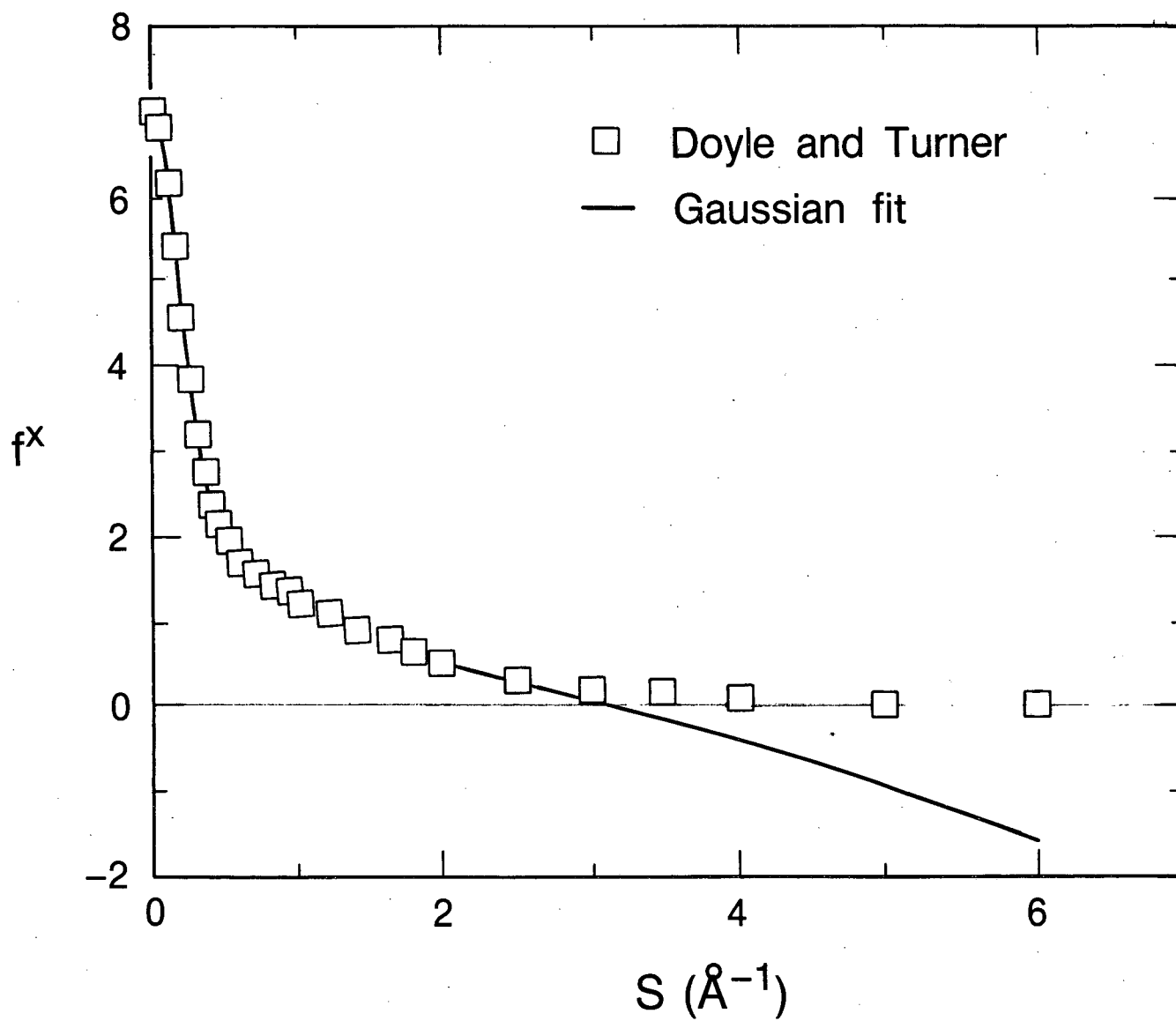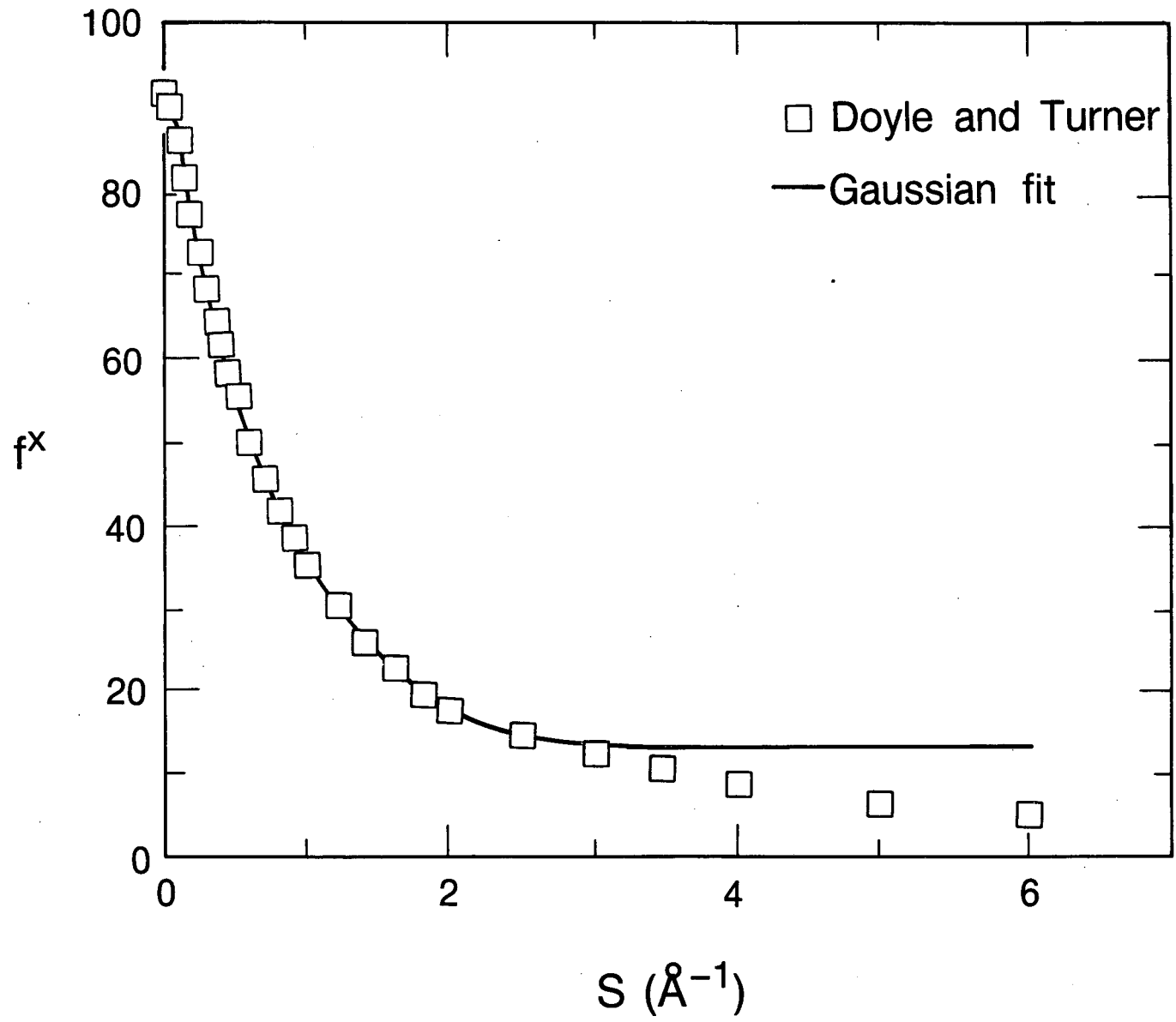
Figure 1(a)

XBL 8811-9793A
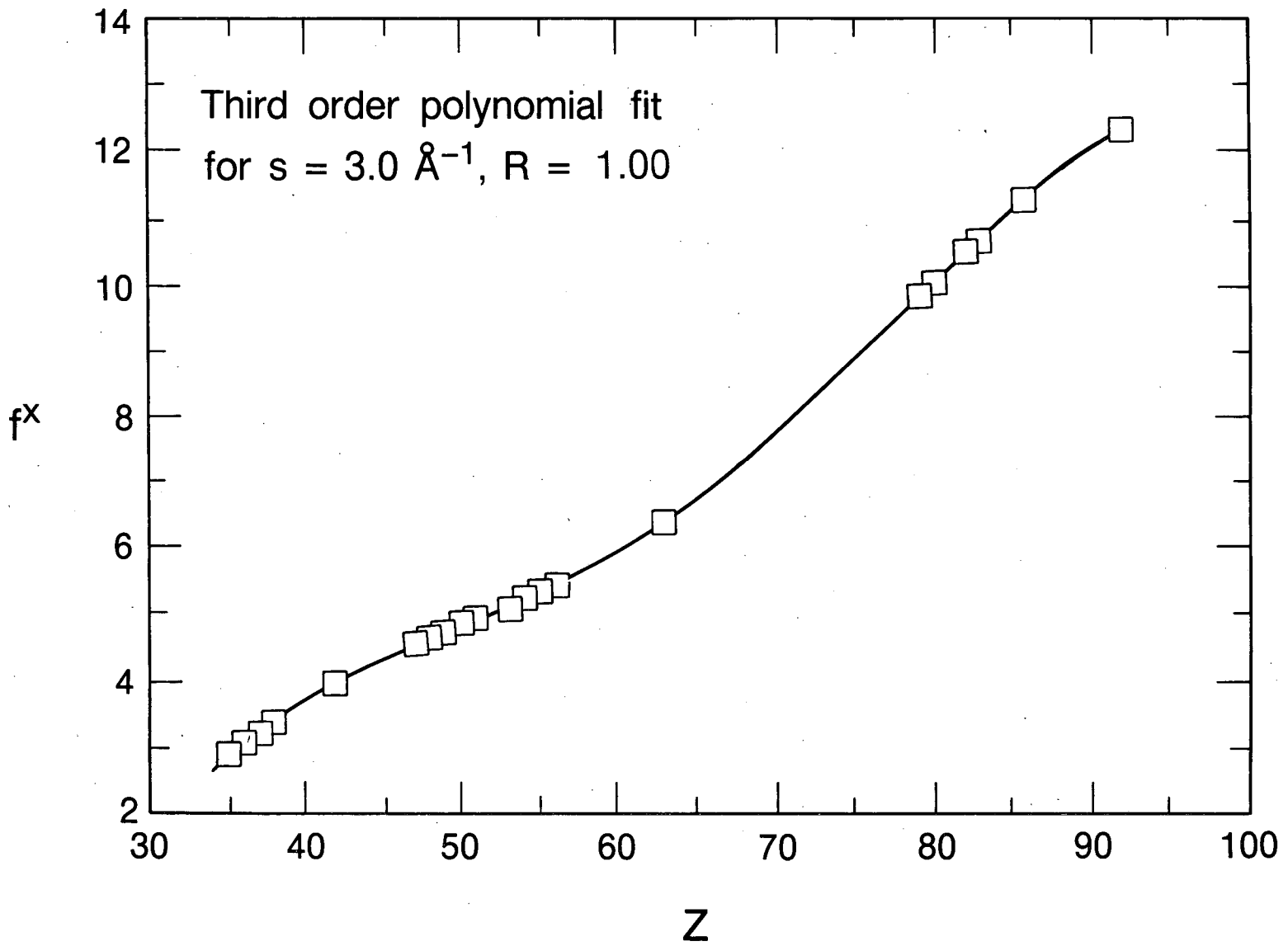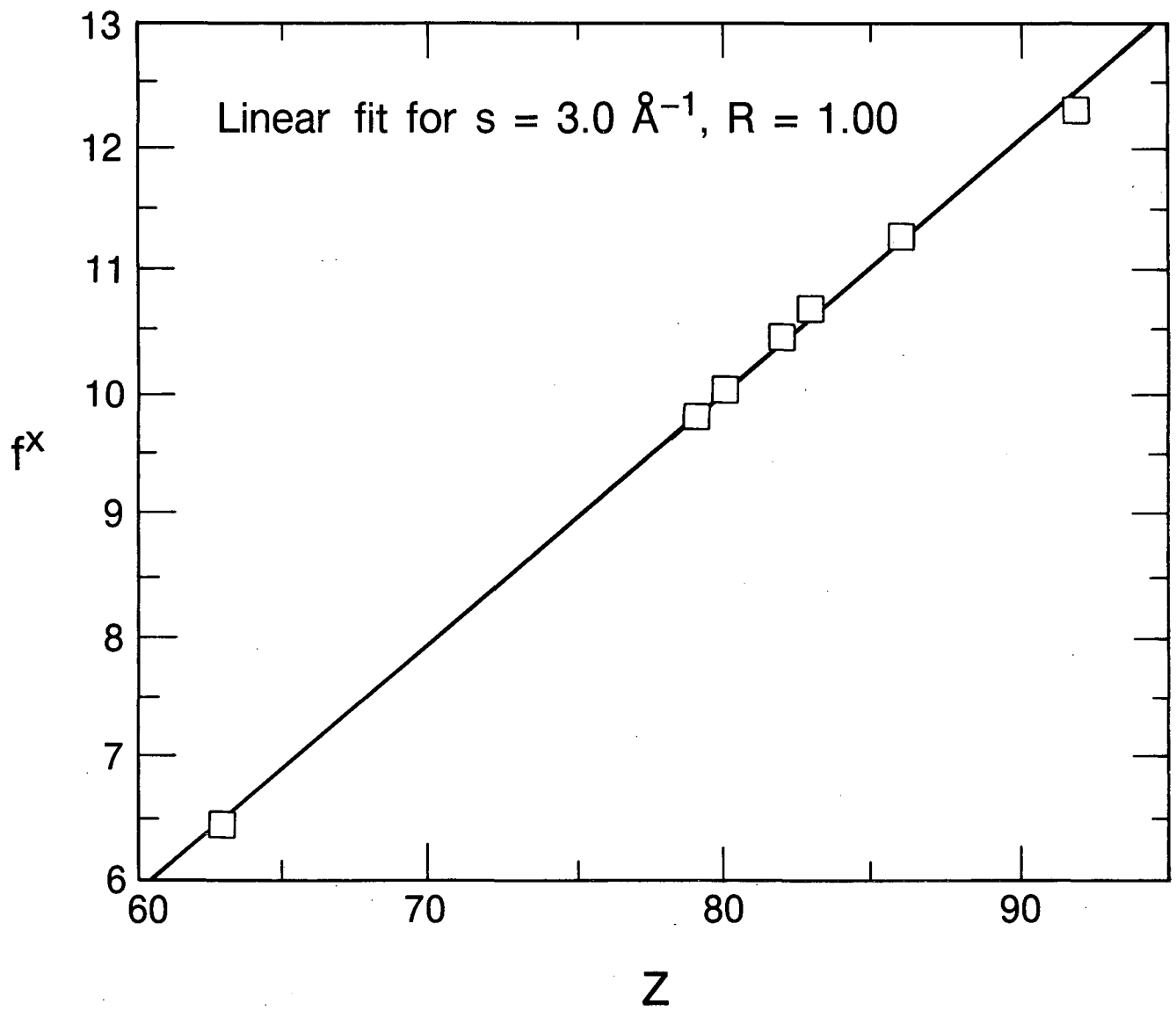
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Figure 1(b)

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Third order polynomial fit for $s = 3.0$ Å^{-1}, $R = 1.00$

Figure 2

Linear fit for s = 3.0 Å^{-1}, R = 1.00

Figure 3

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