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Robust Parameterization of Elastic and Absorptive Electron Atomic Scattering Factors

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Abstract

A robust algorithm and computer program have been developed for the parameterization of elastic and absorptive electron atomic scattering factors. The algorithm is based on a combined modified simulated-annealing and least-squares method, and the computer program works well for fitting both elastic and absorptive atomic scattering factors with five Gaussians. As an application of this program, the elastic electron atomic scattering factors have been parameterized for all neutral atoms and for s up to 6 $Å^{-1}$. Error analysis shows that the present results are considerably more accurate than the previous analytical fits in terms of the mean square value of the deviation between the numerical and fitted scattering factors. Parameterization for absorptive atomic scattering factors has been made for 17 important materials with the zinc blende structure over the temperature range 1 to 1000 K, where appropriate, and for temperature ranges for which accurate Debye–Waller factors are available. For other materials, the parameterization of the absorptive electron atomic scattering factors can be made using the program by supplying the atomic number of the element, the Debye–Waller factor and the acceleration voltage. For ions or when more accurate numerical results for neutral atoms are available, the program can read in the numerical values of the elastic scattering factors and return the parameters for both the elastic and absorptive scattering factors. The computer routines developed have been tested both on computer workstations and desktop PC computers, and will be made freely available *via* electronic mail or on floppy disk upon request.

1. Introduction

For high-energy electron diffraction, the incident electron interacts with a solid *via* an electrostatic Coulomb potential between the incident electron and the electrons and the positively charged nuclei of the solid. The incident electrons may be scattered elastically or inelastically by the solid. In an *elastic collision*, the incident electron does not lose any energy and the solid is left in its original state, *i.e.* $\varphi_f = \varphi_i$ (here the subscripts f and i denote the final and the initial state, respectively). On the other hand, in an *inelastic collision*, the incident electron loses an amount of energy equal to $\Delta E = E_f - E_i$ and the solid is excited from the initial state φ_i to a final state φ_f.

To a good approximation, the effects of inelastic scattering on the elastic scattering may be taken into account by representing the interaction between the incident electron and the solid by a complex potential. This complex potential is usually called the *optical potential*, in analogy with the long-standing use of a complex refractive index for discussing the optical properties of partially absorbing media (Yoshioka, 1957). After an inelastic collision, the incident electron has lost energy while the solid is excited to a higher-energy state. By virtual scattering processes, the electron may regain ΔE and return from the inelastic channel into the elastic state. However, for high-energy electrons, the probability that the inelastically scattered electron reappears in the elastic channel is very small (Rez, 1978). As far as the elastic scattering is concerned, the inelastically scattered electron has been 'absorbed' and the inelastic scattering events contribute only an imaginary addition to the optical potential. For a solid consisting of N atoms, the optical potential may be expressed as a sum of atomic contributions from all atoms:

$$V(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i(\mathbf{r} - \mathbf{r}_i), \tag{1}$$

where the contribution from the ith atom $\varphi_i(\mathbf{r})$ is related to the atomic scattering factor $f^{(e)}(s)$ *via* the following equation:

$$\varphi(\mathbf{r}) = (\hbar^2/m_0\pi) \int f^{(e)}(\mathbf{q}) \exp(4\pi i \mathbf{q} \cdot \mathbf{r})\, d\mathbf{q}, \tag{2}$$

where m_0 is the rest mass of the electron and $\hbar = h/2\pi$, h being Planck's constant.

For a complex optical potential, the electron atomic scattering factor $f^{(e)}(s)$ is a complex quantity. The real part of the scattering factor is called the *elastic scattering factor* and can be calculated using, for example, the relativistic Hartree–Fock atomic wave function (Coulthard, 1967; Doyle & Turner, 1968). The imaginary part of the complex scattering factor is called the *absorptive scattering factor*. It has been shown by several authors

that, for all $\mathbf{g} \neq 0$, the atomic contribution to the absorptive scattering factor is dominated by thermal diffuse scattering (TDS) (Whelan, 1965; Humphreys & Hirsch, 1968; Radi, 1970) and the TDS contribution can be calculated readily following the original formulation of Hall & Hirsch (1965) assuming isotropic Debye–Waller factors and an Einstein model for TDS scattering (Bird & King, 1990; Weickenmeier & Kohl, 1991).

While the numerical values of the scattering factors can be incorporated directly into computer programs for dynamical electron diffraction calculations, there exist many situations where an analytic expression for the scattering factors is desired, as in the case of reflection high-energy electron diffraction (RHEED) (Dudarev, Peng & Whelan, 1995) and the development of tensor methods for the direct determination of structures using high-energy electrons (Peng & Dudarev, 1994*a*,*b*; Peng & Zuo, 1995; Peng, 1995). The most widely used analytical approximation to $f^{(e)}(s)$ nowadays is to fit the scattering factors as a sum of n Gaussians:

$$f^{(e)}(s) = \sum_{i=1}^{n} a_i \exp(-b_i s^2), \tag{3}$$

where a_i and b_i are fitting parameters. This approximation was first introduced by Vand, Eiland & Pepinsky (1957) for the X-ray scattering factor and later by Doyle & Turner (1968) for the real part of the electron scattering factors. In (3), $s = \sin\theta/\lambda$, θ is the angle of scattering and λ the wavelength of the incident electrons.

The first analytical parameterization of the imaginary part or absorptive scattering factors were performed by Dudarev *et al.* (1995). A major difficulty encountered by them and indeed by all parameterizations of atomic scattering factors using such conventional algorithms as the Marquardt–Levenberg procedure is that the results so obtained depend sensitively on the initially assigned values of the fitting parameters. This situation may not seem to be so serious for elastic scattering factors since the number of data sets is limited. But, for absorptive scattering factors, a more robust procedure is needed. This is because, for a given element, the absorptive scattering factors depend on both the angles of scattering and the Debye–Waller factors. It is difficult to make an exhaustive tabulation of all parameters for all elements and compounds. A more sensible approach would be to develop a computer routine that is able to return automatically the required fitting parameters given the name of the element, the acceleration voltage and the Debye–Waller factor. The conventional routines based on the Marquardt–Levenberg algorithm or other minimization procedures do not meet this requirement because to obtain good results from these routines some prior knowledge of the initial values of the fitting parameters is required. In this paper, we aim to develop a robust algorithm and computer routines for the parameterization of the atomic scattering factors and to apply this procedure to obtain accurate parameterization of both the elastic and absorptive atomic scattering factors. By robust, we mean that the procedure should be able to fit a wide range of numerical scattering factors with high accuracy without any human interference, such as an informed guess of the initial values of the fitting parameters.

2. The algorithm

In this section, we seek to develop an algorithm that is stable against any prior assumptions on the initial values of the fitting parameters. The widely used Marquardt–Levenberg or other conventional minimization procedures (Press, Flannery, Teukolsky & Vetterling, 1989) do not meet this criterion, since all these procedures tend to be trapped by local minima as for the parameterization of atomic scattering factors (Rez, Rez & Grant, 1994; Waasmaier & Kirfel, 1995).

Our algorithm is based on a combined modified simulated-annealing procedure (Kirkpatrick, Gelatt & Vecchi, 1983) and the least-squares method for solving linear algebraic equations (Press *et al.*, 1989). The method of simulated annealing is known to be suitable for optimization problems of large scale, especially ones where a desired global minimum is hidden among many, poorer, local minima. The aim of our procedure is to find a set of a_j and b_j that minimizes an objective function (the χ^2 function to be defined below) and gives a best fit of the numerical scattering factors $\{f(s_i)\}$ as a sum of n Gaussians (3).

The procedure starts by assigning random numbers to the initial values of the n fitting parameters b_j ($j = 1, \ldots, n$) in the range $0 < b_j < b_0$, where b_0 is a parameter that controls the area of the parameter space spanned by b_j that is to be searched by the fitting procedure. For a given set of m numerical scattering factors $f(s_i)$ ($i = 1, \ldots, m$), m linear algebraic equations can then be written down for the n free parameters a_j ($j = 1, \ldots, n$):

$$f(s_i) = \sum_{j=1}^{n} a_j \exp(-b_j s_i^2). \tag{4}$$

Equation (4) can be rewritten in matrix form as

$$\mathbf{F} = \mathbf{BA}, \tag{5}$$

where $\mathbf{F}$ is an m-dimensional vector with $(F)_i = f(s_i)$, $\mathbf{A}$ is an n-dimensional parameter vector with $(A)_j = a_j$ and $\mathbf{B}$ is an $m \times n$ matrix with elements $\{B\}_{ij} = \exp(-b_j s_i^2)$. Normally, the number of numerical data points m is much larger than the number n of unknowns and the problem (5) is therefore overdetermined. In general, there exists no solution to the vector $\mathbf{A}$. We can, however, find a compromise solution that comes closest to satisfying all equations simultaneously. Here,

the closeness is defined in the least-squares sense, *i.e.* the sum of the squares of the differences between the left- and right-hand sides of (5) is minimized. The over-determined problem (5) then reduces to a linear least-squares problem. The solution to this linear least-squares problem can be obtained by multiply both sides of (5) by $\mathbf{B}^T$, the transpose of the matrix $\mathbf{B}$

$$(\mathbf{B}^T\mathbf{F}) = (\mathbf{B}^T\mathbf{B})\mathbf{A}. \tag{6}$$

The above equation is called the *normal equation* of the linear least-squares problem (5). Since the matrix $(\mathbf{B}^T\mathbf{B})$ is an $n \times n$ matrix, formally the solution may then be obtained as

$$\mathbf{A} = (\mathbf{B}^T\mathbf{B})^{-1}(\mathbf{B}^T\mathbf{F}). \tag{7}$$

In reality, the $n \times n$ matrix $(\mathbf{B}^T\mathbf{B})$ can be singular giving divergent results. This situation can be avoided by the method of singular-value decomposition (SVD) (see, for example, Press *et al.*, 1989), and this is the method used in our program for solving (5).

Using the solution $\mathbf{A}$, a χ^2 function can be calculated as follows:

$$\chi^2 = \sum_{i=1}^{m} \sigma_i^{-2}\left[f(s_i) - \sum_{j=1}^{n} a_j \exp(-b_j s_i^2)\right]^2, \tag{8}$$

where σ_j^{-2} is usually taken to be the inverse of the variance of the jth 'experimental measurement'. However, in our case, we take this quantity to represent the *density* of the data point as a function of s, *i.e.*

$$\sigma_j^{-2} = \tfrac{1}{2}[s_{j+1} - s_{j-1}]. \tag{9}$$

After χ^2 has been calculated for the given b_j and the a_j obtained from solving (7), the parameters b_j then move randomly towards the next step (here we denote it by b_j^*) according to the rule

$$b_j^* = b_j + (1.0 - r)b_t, \tag{10}$$

where $b_t = b_0 T$, T is a parameter that represents the *temperature* of the system and r is a random number in the range $0.0 < r < 1.0$. For this new set of parameters, b_j^*, another set of linear algebraic equations is set up as for (4) and solved by the SVD method. A new χ^2 is then calculated and compared with the old χ^2. If the new value of χ^2 is lower than the previous value, the parameters b_j are then updated to b_j^*. Otherwise, new b_j^* are tried according to (10). This process is continued until the total number of random walks that do not improve the χ^2 value excceeds a certain number (say 200). The temperature is then decreased according to the law $T \rightarrow T\delta t$, in which δt is a parameter in the range 0.9 to 0.999, and consequently the step b_t for the random walk of b_j is reduced. The process is finally terminated if the temperature is decreased to less than a threshold temperature (say 0.05).

The analogy of the present procedure with thermodynamics, especially with the way that liquids freeze and crystallize, is to be noted. At high temperatures (high T), the molecules of a liquid move freely with respect with each other (large b_t). If the liquid is cooled slowly ($T \rightarrow T\delta t$), the thermal mobility of the molecules is lost gradually ($b_t = b_0 T$ decreases with T). If the cooling process is very slow so that atoms have ample time to redistribute themselves as they lose mobility, the atoms are then able to line themselves up and form a pure crystal at low temperature. The crystal so formed is then in a state of minimum energy for the system (with a global minimum of χ^2).

3. Computer routines and results

A Fortran routine *MCFIT* for the analytical fitting of numerical scattering factors using n Gaussians (3) is developed based on the algorithm described in the previous section. In this paper, the number of Gaussians is taken to be 5; using this number, we found satisfactory results for both the elastic and the absorptive scattering factors. The accuracy of the routine is controlled by three parameters, the initial temperature T_0, the initial step b_0 for the random walk of b_j, and the parameter δt that determines how the temperature decreases. To improve the efficiency of the routine, the procedure is first applied only to a subset of the complete data set (one tenth). The resulting values for the fitting parameters a_j and b_j are then taken as the initial values for a more through search using the complete numerical data set.

The parameter b_0 determines the area within the parameter space spanned by b_j ($j = 1, \ldots, 5$) that is to be searched by the routine *MCFIT*. In principle, if the search is exhaustive (*i.e.* b_0 is large enough), the initial temperature T_0 is high enough and the system is cooled down sufficiently slowly ($\delta t \rightarrow 1.0$), the modified simulated-annealing algorithm as described in the previous section will find a unique set of parameters a_j, b_j, giving a global minimum of χ^2. For finite values of b_0, T_0 and δt, the algorithm is only approximate in the sense that only a subspace of the true parameter space will be searched by the algorithm and the system might not be in the ground state of minimum energy when the system is cooled to zero temperature, in analogy with a quenching process in which a liquid does not reach a crystalline state but rather ends up in a polycrystalline or amorphous state having somewhat higher energy.

Fortunately for the parameterization of the atomic scattering factors, we do not have to find the true global minimum. The controlling parameters are therefore chosen as a result of compromise between the desired accuracy and computer time needed to achieve such an accuracy. Our experience shows that very respectable results may be obtained for $b_0 = 1.0$, $T_0 = 1.0$ and

Table 1. *Elastic scattering factors for s up to 2.0 Å^{-1}*

Element	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5
H	1	0.0349	0.1201	0.1970	0.0573	0.1195	0.5347	3.5867	12.3471	18.9525	38.6269
He	2	0.0317	0.0838	0.1526	0.1334	0.0164	0.2507	1.4751	4.4938	12.6646	31.1653
Li	3	0.0750	0.2249	0.5548	1.4954	0.9354	0.3864	2.9383	15.3829	53.5545	138.7337
Be	4	0.0780	0.2210	0.6740	1.3867	0.6925	0.3131	2.2381	10.1517	30.9061	78.3273
B	5	0.0909	0.2551	0.7738	1.2136	0.4606	0.2995	2.1155	8.3816	24.1292	63.1314
C	6	0.0893	0.2563	0.7570	1.0487	0.3575	0.2465	1.7100	6.4094	18.6113	50.2523
N	7	0.1022	0.3219	0.7982	0.8197	0.1715	0.2451	1.7481	6.1925	17.3894	48.1431
O	8	0.0974	0.2921	0.6910	0.6990	0.2039	0.2067	1.3815	4.6943	12.7105	32.4726
F	9	0.1083	0.3175	0.6487	0.5846	0.1421	0.2057	1.3439	4.2788	11.3932	28.7881
Ne	10	0.1269	0.3535	0.5582	0.4674	0.1460	0.2200	1.3779	4.0203	9.4934	23.1278
Na	11	0.2142	0.6853	0.7692	1.6589	1.4482	0.3334	2.3446	10.0830	48.3037	138.2700
Mg	12	0.2314	0.6866	0.9677	2.1882	1.1339	0.3278	2.2720	10.9241	39.2898	101.9748
Al	13	0.2390	0.6573	1.2011	2.5586	1.2312	0.3138	2.1063	10.4163	34.4552	98.5344
Si	14	0.2519	0.6372	1.3795	2.5082	1.0500	0.3075	2.0174	9.6746	29.3744	80.4732
P	15	0.2548	0.6106	1.4541	2.3204	0.8477	0.2908	1.8740	8.5176	24.3434	63.2996
S	16	0.2497	0.5628	1.3899	2.1865	0.7715	0.2681	1.6711	7.0267	19.5377	50.3888
Cl	17	0.2443	0.5397	1.3919	2.0197	0.6621	0.2468	1.5242	6.1537	16.6687	42.3086
Ar	18	0.2385	0.5017	1.3428	1.8899	0.6079	0.2289	1.3694	5.2561	14.0928	35.5361
K	19	0.4115	1.4031	2.2784	2.6742	2.2162	0.3703	3.3874	13.1029	68.9592	194.4329
Ca	20	0.4054	1.3880	2.1602	3.7532	2.2063	0.3499	3.0991	11.9608	53.9353	142.3892
Sc	21	0.3787	1.2181	2.0594	3.2618	2.3870	0.3133	2.5856	9.5813	41.7688	116.7282
Ti	22	0.3825	1.2598	2.0008	3.0617	2.0694	0.3040	2.4863	9.2783	39.0751	109.4583
V	23	0.3876	1.2750	1.9109	2.8314	1.8979	0.2967	2.3780	8.7981	35.9528	101.7201
Cr	24	0.4046	1.3696	1.8941	2.0800	1.2196	0.2986	2.3958	9.1406	37.4701	113.7121
Mn	25	0.3796	1.2094	1.7815	2.5420	1.5937	0.2699	2.0455	7.4726	31.0604	91.5622
Fe	26	0.3946	1.2725	1.7031	2.3140	1.4795	0.2717	2.0443	7.6007	29.9714	86.2265
Co	27	0.4118	1.3161	1.6493	2.1930	1.2830	0.2742	2.0372	7.7205	29.9680	84.9383
Ni	28	0.3860	1.1765	1.5451	2.0730	1.3814	0.2478	1.7660	6.3107	25.2204	74.3146
Cu	29	0.4314	1.3208	1.5236	1.4671	0.8562	0.2694	1.9223	7.3474	28.9892	90.6246
Zn	30	0.4288	1.2646	1.4472	1.8294	1.0934	0.2593	1.7998	6.7500	25.5860	73.5284
Ga	31	0.4818	1.4032	1.6561	2.4605	1.1054	0.2825	1.9785	8.7546	32.5238	98.5523
Ge	32	0.4655	1.3014	1.6088	2.6998	1.3003	0.2647	1.7926	7.6071	26.5541	77.5238
As	33	0.4517	1.2229	1.5852	2.7958	1.2638	0.2493	1.6436	6.8154	22.3681	62.0390
Se	34	0.4477	1.1678	1.5843	2.8087	1.1956	0.2405	1.5442	6.3231	19.4610	52.0233
Br	35	0.4798	1.1948	1.8695	2.6953	0.8203	0.2504	1.5963	6.9653	19.8492	50.3233
Kr	36	0.4546	1.0993	1.7696	2.7068	0.8672	0.2309	1.4279	5.9449	16.6752	42.2243
Rb	37	1.0160	2.8528	3.5466	-7.7804	12.1148	0.4853	5.0925	25.7851	130.4515	138.6775
Sr	38	0.6703	1.4926	3.3368	4.4600	3.1501	0.3190	2.2287	10.3504	52.3291	151.2216
Y	39	0.6894	1.5474	3.2450	4.2126	2.9764	0.3189	2.2904	10.0062	44.0771	125.0120
Zr	40	0.6719	1.4684	3.1668	3.9557	2.8920	0.3036	2.1249	8.9236	36.8458	108.2049
Nb	41	0.6123	1.2677	3.0348	3.3841	2.3683	0.2709	1.7683	7.2489	27.9465	98.5624
Mo	42	0.6773	1.4798	3.1788	3.0824	1.8384	0.2920	2.0606	8.1129	30.5336	100.0658
Tc	43	0.7082	1.6392	3.1993	3.4327	1.8711	0.2976	2.2106	8.5246	33.1456	96.6377
Ru	44	0.6735	1.4934	3.0966	2.7254	1.5597	0.2773	1.9716	7.3249	26.6891	90.5581
Rh	45	0.6413	1.3690	2.9854	2.6952	1.5433	0.2580	1.7721	6.3854	23.2549	85.1517
Pd	46	0.5904	1.1775	2.6519	2.2875	0.8689	0.2324	1.5019	5.1591	15.5428	46.8213
Ag	47	0.6377	1.3790	2.8294	2.3631	1.4553	0.2466	1.6974	5.7656	20.0943	76.7372
Cd	48	0.6364	1.4247	2.7802	2.5973	1.7886	0.2407	1.6823	5.6588	20.7219	69.1109
In	49	0.6768	1.6589	2.7740	3.1835	2.1326	0.2522	1.8545	6.2936	25.1457	84.5448
Sn	50	0.7224	1.9610	2.7161	3.5603	1.8972	0.2651	2.0604	7.3011	27.5493	81.3349
Sb	51	0.7106	1.9247	2.6149	3.8322	1.8899	0.2562	1.9646	6.8852	24.7648	68.9168
Te	52	0.6947	1.8690	2.5356	4.0013	1.8955	0.2459	1.8542	6.4411	22.1730	59.2206
I	53	0.7047	1.9484	2.5940	4.1526	1.5057	0.2455	1.8638	6.7639	21.8007	56.4395
Xe	54	0.6737	1.7908	2.4129	4.2100	1.7058	0.2305	1.6890	5.8218	18.3928	47.2496
Cs	55	1.2704	3.8018	5.6618	0.9205	4.8105	0.4356	4.2058	23.4342	136.7783	171.7561
Ba	56	0.9049	2.6076	4.8498	5.1603	4.7388	0.3066	2.4363	12.1821	54.6135	161.9978
La	57	0.8405	2.3863	4.6139	5.1514	4.7949	0.2791	2.1410	10.3400	41.9148	132.0204
Ce	58	0.8551	2.3915	4.5772	5.0278	4.5118	0.2805	2.1200	10.1808	42.0633	130.9893
Pr	59	0.9096	2.5313	4.5266	4.6376	4.3690	0.2939	2.2471	10.8266	48.8842	147.6020
Nd	60	0.8807	2.4183	4.4448	4.6858	4.1725	0.2802	2.0836	10.0357	47.4506	146.9976
Pm	61	0.9471	2.5463	4.3523	4.4789	3.9080	0.2977	2.2276	10.5762	49.3619	145.3580
Sm	62	0.9699	2.5837	4.2778	4.4575	3.5985	0.3003	2.2447	10.6487	50.7994	146.4179
Eu	63	0.8694	2.2413	3.9196	3.9694	4.5498	0.2653	1.8590	8.3998	36.7397	125.7089
Gd	64	0.9673	2.4702	4.1148	4.4972	3.2099	0.2909	2.1014	9.7067	43.4270	125.9474
Tb	65	0.9325	2.3673	3.8791	3.9674	3.7996	0.2761	1.9511	8.9296	41.5937	131.0122
Dy	66	0.9505	2.3705	3.8218	4.0471	3.4451	0.2773	1.9469	8.8862	43.0938	133.1396

Table 1. *(cont.)*

Element	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5
Ho	67	0.9248	2.2428	3.6182	3.7910	3.7912	0.2660	1.8183	7.9655	33.1129	101.8139
Er	68	1.0373	2.4824	3.6558	3.8925	3.0056	0.2944	2.0797	9.4156	45.8056	132.7720
Tm	69	1.0075	2.3787	3.5440	3.6932	3.1759	0.2816	1.9486	8.7162	41.8420	125.0320
Yb	70	1.0347	2.3911	3.4619	3.6556	3.0052	0.2855	1.9679	8.7619	42.3304	125.6499
Lu	71	0.9927	2.2436	3.3554	3.7813	3.0994	0.2701	1.8073	7.8112	34.4849	103.3526
Hf	72	1.0295	2.2911	3.4110	3.9497	2.4925	0.2761	1.8625	8.0961	34.2712	98.5295
Ta	73	1.0190	2.2291	3.4097	3.9252	2.2679	0.2694	1.7962	7.6944	31.0942	91.1089
W	74	0.9853	2.1167	3.3570	3.7981	2.2798	0.2569	1.6745	7.0098	26.9234	81.3910
Re	75	0.9914	2.0858	3.4531	3.8812	1.8526	0.2548	1.6518	6.8845	26.7234	81.7215
Os	76	0.9813	2.0322	3.3665	3.6235	1.9741	0.2487	1.5973	6.4737	23.2817	70.9254
Ir	77	1.0194	2.0645	3.4425	3.4914	1.6976	0.2554	1.6475	6.5966	23.2269	70.0272
Pt	78	0.9148	1.8096	3.2134	3.2953	1.5754	0.2263	1.3813	5.3243	17.5987	60.0171
Au	79	0.9674	1.8916	3.3993	3.0524	1.2607	0.2358	1.4712	5.6758	18.7119	61.5286
Hg	80	1.0033	1.9469	3.4396	3.1548	1.4180	0.2413	1.5298	5.8009	19.4520	60.5753
Tl	81	1.0689	2.1038	3.6039	3.4927	1.8283	0.2540	1.6715	6.3509	23.1531	78.7099
Pb	82	1.0891	2.1867	3.6160	3.8031	1.8994	0.2552	1.7174	6.5131	23.9170	74.7039
Bi	83	1.1007	2.2306	3.5689	4.1549	2.0382	0.2546	1.7351	6.4948	23.6464	70.3780
Po	84	1.1568	2.4353	3.6459	4.4064	1.7179	0.2648	1.8786	7.1749	25.1766	69.2821
At	85	1.0909	2.1976	3.3831	4.6700	2.1277	0.2466	1.6707	6.0197	20.7657	57.2663
Rn	86	1.0756	2.1630	3.3178	4.8852	2.0489	0.2402	1.6169	5.7644	19.4568	52.5009
Fr	87	1.4282	3.5081	5.6767	4.1964	3.8946	0.3183	2.6889	13.4816	54.3866	200.8321
Ra	88	1.3127	3.1243	5.2988	5.3891	5.4133	0.2887	2.2897	10.8276	43.5389	145.6109
Ac	89	1.3128	3.1021	5.3385	5.9611	4.7562	0.2861	2.2509	10.5287	41.7796	128.2973
Th	90	1.2553	2.9178	5.0862	6.1206	4.7122	0.2701	2.0636	9.3051	34.5977	107.9200
Pa	91	1.3218	3.1444	5.4371	5.6444	4.0107	0.2827	2.2250	10.2454	41.1162	124.4449
U	92	1.3382	3.2043	5.4558	5.4839	3.6342	0.2838	2.2452	10.2519	41.7251	124.9023
Np	93	1.5193	4.0053	6.5327	−0.1402	6.7489	0.3213	2.8206	14.8878	68.9103	81.7257
Pu	94	1.3517	3.2937	5.3213	4.6466	3.5714	0.2813	2.2418	9.9952	42.7939	132.1739
Am	95	1.2135	2.7962	4.7545	4.5731	4.4786	0.2483	1.8437	7.5421	29.3841	112.4579
Cm	96	1.2937	3.1100	5.0393	4.7546	3.5031	0.2638	2.0341	8.7101	35.2992	109.4972
Bk	97	1.2915	3.1023	4.9309	4.6009	3.4661	0.2611	2.0023	8.4377	34.1559	105.8911
Cf	98	1.2089	2.7391	4.3482	4.0047	4.6497	0.2421	1.7487	6.7262	23.2153	80.3108

$\delta t = 0.9$. The CPU time spent for a typical run is about 1 min on an HP735 computer workstation. Much improved results may be obtained using $b_0 = 4.0$, $T_0 = 3.0$ and $\delta t = 0.99$. The CPU time for a typical run is about 2 min for these parameters. Very accurate results may be obtained using $T_0 = 30$, $b_0 = 1$, $\delta t = 0.99$.

Two Fortran computer programs have been developed using the routine *MCFIT* for fitting the elastic and the absorptive atomic scattering factors. The first program, *ELAS*98, reads a data file that contains all the numerical values of elastic scattering factors for all 98 neutral elements and returns n pairs of a_j, b_j. The results are given in Table 1 for the range $s = 0 \rightarrow 2\,\text{Å}^{-1}$ and in Table 3 for the range $s = 0 \rightarrow 6\,\text{Å}^{-1}$. Previously, parameterization of the electron elastic scattering factors has been made by Doyle & Turner (1968) for some selected neutral elements and ions for the range $s = 0 \rightarrow 2\,\text{Å}^{-1}$. A more complete parameterization for all neutral elements has been made by Jiang & Li (1984) for the same range of s values. Unfortunately, the paper by Jiang & Li was published in Chinese and their results are not widely known outside China.

Parameterization using a different analytic approximating to the numerical scattering factors for the full range of s was published by Weickenmeier & Kohl (1991) for all neutral elements. Numerical values for the same angular range can also be obtained using the computer routine of Bird & King (1990). In Tables 2 and 4, we have listed the root of the mean square value of the deviation σ^2 between the numerical and fitted scattering factors using the parameters given in Tables 1 and 3:

$$\sigma = \left\{ \sum_{i=1}^{m} (1/m) \left[f(s_i) - \sum_{j=1}^{5} a_j \exp(-b_j s_i) \right]^2 \right\}^{1/2}, \tag{11}$$

and an E factor [the root of the mean square expressed as a percentage of $f(0)$] for each element as defined by Doyle & Turner (1968),

$$E = [100/f(0)]\sigma, \tag{12}$$

and these factors (denoted in the tables as PRDW) have been compared with those obtained using the parameterization of Weickenmeier & Kohl (1991) (denoted by WK), the numerical routine of Bird & King (1990) (denoted by BK) and the analytical fitting of Doyle & Turner (denoted by DT).

Results for WK were obtained using the routines *GETWK* and *WEKO* extracted from the computer program *FSCATT* kindly provided by Dr Weickenmeier.

Table 2. *Error analysis of Table 1*

In the table WK denotes Weickenmeier & Kohl (1991); DT denotes Doyle & Turner (1968), BK denotes Bird & King (1990) and PRDW denotes Peng, Ren, Dudarev & Whelan (this paper).

		WK		DT		BK		PRDW	
Element	Z	σ	E	σ	E	σ	E	σ	E
H	1					0.0017	0.3179	0.0012	0.2240
He	2	0.0087	2.0883	0.0003	0.0769	0.0003	0.0787	0.0003	0.0667
Li	3	0.0090	0.2735	0.0036	0.1082	0.0049	0.1507	0.0007	0.0225
Be	4	0.0082	0.2673	0.0024	0.0773	0.0012	0.0377	0.0005	0.0158
B	5	0.0139	0.4961	0.0019	0.0698	0.0007	0.0243	0.0004	0.0126
C	6	0.0116	0.4617	0.0016	0.0620	0.0004	0.0175	0.0004	0.0144
N	7	0.0041	0.1848	0.0018	0.0821	0.0014	0.0622	0.0012	0.0523
O	8	0.0166	0.8354	0.0008	0.0414	0.0003	0.0160	0.0003	0.0149
F	9	0.0023	0.1271	0.0006	0.0350	0.0003	0.0178	0.0003	0.0150
Ne	10	0.0029	0.1747	0.0005	0.0300	0.0003	0.0198	0.0003	0.0162
Na	11	0.0295	0.6164	0.0073	0.1522	0.0073	0.1536	0.0016	0.0325
Mg	12	0.0450	0.8651	0.0058	0.1107	0.0028	0.0541	0.0011	0.0216
Al	13	0.0580	0.9841	0.0068	0.1158	0.0027	0.0455	0.0013	0.0218
Si	14	0.0240	0.4126	0.0056	0.0963	0.0018	0.0316	0.0009	0.0163
P	15	0.0228	0.4162	0.0042	0.0757	0.0012	0.0225	0.0008	0.0145
S	16	0.0166	0.3224	0.0032	0.0616	0.0010	0.0203	0.0005	0.0106
Cl	17	0.0499	1.0277	0.0025	0.0518	0.0006	0.0115	0.0004	0.0089
Ar	18	0.0442	0.9658	0.0020	0.0435	0.0004	0.0093	0.0004	0.0090
K	19	0.0323	0.3591	0.0164	0.1821	0.0242	0.2694	0.0034	0.0378
Ca	20	0.0961	0.9696	0.0136	0.1376	0.0120	0.1207	0.0029	0.0293
Sc	21	0.0814	0.8746	0.0123	0.1321	0.0078	0.0842	0.0022	0.0240
Ti	22	0.0210	0.2393	0.0114	0.1297	0.0059	0.0672	0.0021	0.0239
V	23	0.0309	0.3723	0.0106	0.1271	0.0046	0.0548	0.0019	0.0232
Cr	24	0.0908	1.3024	0.0100	0.1432	0.0035	0.0509	0.0019	0.0268
Mn	25	0.0302	0.4029	0.0092	0.1226	0.0030	0.0398	0.0018	0.0246
Fe	26	0.0331	0.4617	0.0087	0.1208	0.0025	0.0343	0.0016	0.0222
Co	27	0.0606	0.8843	0.0081	0.1182	0.0021	0.0307	0.0014	0.0207
Ni	28	0.0442	0.6733	0.0076	0.1152	0.0018	0.0272	0.0046	0.0697
Cu	29	0.0718	1.2818	0.0073	0.1302	0.0015	0.0268	0.0013	0.0226
Zn	30	0.0487	0.8029	0.0066	0.1088	0.0013	0.0220	0.0011	0.0189
Ga	31	0.0509	0.7167	0.0096	0.1349	0.0025	0.0349	0.0017	0.0234
Ge	32	0.0818	1.1090	0.0082	0.1117	0.0019	0.0251	0.0015	0.0206
As	33	0.0477	0.6521	0.0065	0.0886	0.0014	0.0186	0.0012	0.0160
Se	34	0.0137	0.1895	0.0051	0.0714	0.0013	0.0181	0.0009	0.0121
Br	35	0.0276	0.3905	0.0043	0.0611	0.0011	0.0157	0.0007	0.0102
Kr	36	0.0268	0.3881	0.0037	0.0537	0.0008	0.0113	0.0006	0.0084
Rb	37	0.1089	0.9247	0.0247	0.2097	0.0327	0.2777	0.0211	0.1793
Sr	38	0.0583	0.4449	0.0225	0.1713	0.0190	0.1448	0.0051	0.0390
Y	39	0.1211	0.9556			0.0097	0.0764	0.0039	0.0307
Zr	40	0.0924	0.7593			0.0067	0.0547	0.0038	0.0312
Nb	41	0.0981	0.9183			0.0450	0.4210	0.0045	0.0422
Mo	42	0.0903	0.8799	0.0143	0.1391	0.0042	0.0409	0.0027	0.0268
Tc	43	0.0736	0.6781			0.0030	0.0279	0.0029	0.0264
Ru	44	0.0852	0.8910			0.0025	0.0262	0.0027	0.0283
Rh	45	0.0840	0.9087			0.0022	0.0233	0.0028	0.0303
Pd	46	0.0450	0.5934			0.0019	0.0250	0.0019	0.0254
Ag	47	0.1011	1.1661	0.0105	0.1208	0.0020	0.0228	0.0034	0.0397
Cd	48	0.0548	0.5934	0.0100	0.1084	0.0018	0.0198	0.0028	0.0303
In	49	0.0968	0.9282	0.0139	0.1329	0.0034	0.0330	0.0042	0.0402
Sn	50	0.1138	1.0482	0.0123	0.1132	0.0028	0.0255	0.0024	0.0217
Sb	51	0.0646	0.5890	0.0103	0.0941	0.0023	0.0213	0.0019	0.0171
Te	52	0.0272	0.2473			0.0025	0.0225	0.0019	0.0169
I	53	0.0703	0.6450	0.0076	0.0699	0.0020	0.0183	0.0012	0.0111
Xe	54	0.0338	0.3133	0.0064	0.0596	0.0016	0.0150	0.0011	0.0104
Cs	55	0.1772	1.0737	0.0356	0.2158	0.0514	0.3111	0.0297	0.1798
Ba	56	0.0692	0.3786	0.0347	0.1897	0.0347	0.1900	0.0065	0.0353
La	57	0.0973	0.5465			0.0175	0.0982	0.0066	0.0371
Ce	58	0.0976	0.5619			0.0150	0.0864	0.0061	0.0350
Pr	59	0.0802	0.4723			0.0177	0.1040	0.0065	0.0383
Nd	60	0.0834	0.5024			0.0183	0.1101	0.0063	0.0376
Pm	61	0.0836	0.5147			0.0158	0.0974	0.0059	0.0362
Sm	62	0.0806	0.5071			0.0159	0.0999	0.0060	0.0380
Eu	63	0.1252	0.8046	1.3898	8.9302	0.0194	0.1245	0.0073	0.0467

Table 2. *(cont.)*

		WK		DT		BK		PRDW	
Element	Z	σ	E	σ	E	σ	E	σ	E
Gd	64	0.0580	0.3801			0.0117	0.0766	0.0049	0.0321
Tb	65	0.1003	0.6695			0.0119	0.0796	0.0077	0.0514
Dy	66	0.0927	0.6334			0.0127	0.0871	0.0058	0.0396
Ho	67	0.0425	0.2957			0.0086	0.0600	0.0051	0.0355
Er	68	0.1048	0.7445			0.0122	0.0869	0.0051	0.0362
Tm	69	0.0436	0.3157			0.0095	0.0686	0.0053	0.0382
Yb	70	0.0476	0.3509			0.0100	0.0734	0.0044	0.0324
Lu	71	0.0424	0.3141			0.0075	0.0552	0.0044	0.0323
Hf	72	0.0467	0.3542			0.0072	0.0550	0.0037	0.0277
Ta	73	0.1364	1.0612			0.0044	0.0343	0.0035	0.0269
W	74	0.0573	0.4568			0.0029	0.0228	0.0036	0.0284
Re	75	0.1282	1.0452			0.0024	0.0195	0.0031	0.0253
Os	76	0.0862	0.7189			0.0039	0.0324	0.0030	0.0249
Ir	77	0.0991	0.8457			0.0023	0.0199	0.0023	0.0194
Pt	78	0.0769	0.7114			0.0025	0.0227	0.0034	0.0312
Au	79	0.0631	0.5969	0.0100	0.0949	0.0012	0.0116	0.0019	0.0181
Hg	80	0.0678	0.6180	0.0100	0.0916	0.0014	0.0128	0.0017	0.0159
Tl	81	0.1087	0.8974			0.0034	0.0284	0.0035	0.0291
Pb	82	0.0663	0.5262	0.0144	0.1141	0.0024	0.0192	0.0028	0.0221
Bi	83	0.1024	0.7817	0.0138	0.1052	0.0026	0.0198	0.0025	0.0194
Po	84	0.0604	0.4516			0.0028	0.0207	0.0029	0.0215
At	85	0.0530	0.3937			0.0026	0.0191	0.0019	0.0142
Rn	86	0.0459	0.3402	0.2162	1.6024	0.0022	0.0163	0.0018	0.0133
Fr	87	0.1637	0.8747			0.0280	0.1497	0.0093	0.0495
Ra	88	0.1681	0.8177			0.0227	0.1103	0.0086	0.0418
Ac	89	0.1136	0.5545			0.0168	0.0819	0.0067	0.0329
Th	90	0.1378	0.6852			0.0112	0.0558	0.0065	0.0322
Pa	91	0.1082	0.5530			0.0116	0.0592	0.0058	0.0297
U	92	0.1743	0.9119	0.0307	0.1605	0.0141	0.0737	0.0056	0.0292
Np	93	0.1141	0.6084			0.0121	0.0646	0.0302	0.1611
Pu	94	0.1454	0.7994			0.0127	0.0698	0.0058	0.0321
Am	95	0.1367	0.7661			0.0131	0.0736	0.0091	0.0510
Cm	96	0.2039	1.1514			0.0086	0.0485	0.0051	0.0288
Bk	97	0.1648	0.9466			0.0068	0.0391	0.0052	0.0297
Cf	98	0.1756	1.0428			0.0127	0.0757	0.0225	0.1333

Although in principle the WK fitting would provide the correct asymptotic form for electron scattering factors at large angles of scattering, Tables 2 and 4 show that for the range of s up to $6.0\,\text{Å}^{-1}$ the WK fitting is not as accurate as our fit using five Gaussians in terms of σ and E factors for all neutral atoms.

Results for DT were obtained using the parameters listed in Table 4(*a*) of Doyle & Turner (1968). The E factors listed in Table 2 are slightly different from those listed by Doyle & Turner (1968) in Table 4(*a*). This is because when Doyle & Turner calculated their E factors they used 201 data points rather than the 56 values listed in *International Tables for Crystallography* (Cowley, 1992). Tables 2 and 4 show that for all the 54 elements listed by Doyle & Turner in Table 4(*a*), our results are superior in terms of σ and E factors. It should also be noted that for elements Eu and Rn with atomic numbers 63 and 86, the DT E factors are anomalously large compared with all other elements and also the original Doyle & Turner values. This fact suggests that there are some misprints associated with the fitting parameters listed in Table 4(*a*) of Doyle & Turner (1968). Comparing Tables 2 and 4, we can also conclude that, although the σ and E factors for the full range of s up to $6\,\text{Å}^{-1}$ (Table 3) are systematically larger than that for the range of s up to $2.0\,\text{Å}^{-1}$, these values are certainly not divergent. This situation is unlike that for the X-ray scattering factors for which Fox, O'Keefe & Tabbernor (1989) found that Table 3 of Doyle & Turner (1968) is only applicable to the angular range $s = 0 \rightarrow 2\,\text{Å}^{-1}$ and attempts to extend it to higher angles can lead to large errors. Our Table 4 suggests, however, that respectable results may be obtained for electron scattering factors for s up to $6\,\text{Å}^{-1}$ using the fitting parameters listed in Table 4(*a*) of Doyle & Turner (1968).

Comparison with BK was made using the computer routine *ATOM* kindly provided by Dr Bird. For all elements, the accuracy of their numerical atomic scattering factors is about the same order of magnitude as our analytical fitting. For 17 elements among the 98 neutral elements, their numerical results are superior to our fitting for the range $s = 0 \rightarrow 2\,\text{Å}^{-1}$ (Table 2). For the full range of s up to $6\,\text{Å}^{-1}$, there exist 74 neutral elements for which the BK results are superior to our analytical fitting (Table 4). It should be pointed out that errors

Table 3. *Elastic scattering factors for s up to 6.0 Å^{-1}*

Element	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5
H	1	0.0088	0.0449	0.1481	0.2356	0.0914	0.1152	1.0867	4.9755	16.5591	43.2743
He	2	0.0084	0.0443	0.1314	0.1671	0.0666	0.0596	0.5360	2.4274	7.7852	20.3126
Li	3	0.0478	0.2048	0.5253	1.5225	0.9853	0.2258	2.1032	12.9349	50.7501	136.6280
Be	4	0.0423	0.1874	0.6019	1.4311	0.7891	0.1445	1.4180	8.1165	27.9705	74.8684
B	5	0.0436	0.1898	0.6788	1.3273	0.5544	0.1207	1.1595	6.2474	21.0460	59.3619
C	6	0.0489	0.2091	0.7537	1.1420	0.3555	0.1140	1.0825	5.4281	17.8811	51.1341
N	7	0.0267	0.1328	0.5301	1.1020	0.4215	0.0541	0.5165	2.8207	10.6297	34.3764
O	8	0.0365	0.1729	0.5805	0.8814	0.3121	0.0652	0.6184	2.9449	9.6298	28.2194
F	9	0.0382	0.1822	0.5972	0.7707	0.2130	0.0613	0.5753	2.6858	8.8214	25.6668
Ne	10	0.0380	0.1785	0.5494	0.6942	0.1918	0.0554	0.5087	2.2639	7.3316	21.6912
Na	11	0.1260	0.6442	0.8893	1.8197	1.2988	0.1684	1.7150	8.8386	50.8265	147.2073
Mg	12	0.1130	0.5575	0.9046	2.1580	1.4735	0.1356	1.3579	6.9255	32.3165	92.1138
Al	13	0.1165	0.5504	1.0179	2.6295	1.5711	0.1295	1.2619	6.8242	28.4577	88.4750
Si	14	0.0567	0.3365	0.8104	2.4960	2.1186	0.0582	0.6155	3.2522	16.7929	57.6767
P	15	0.1005	0.4615	1.0663	2.5854	1.2725	0.0977	0.9084	4.9654	18.5471	54.3648
S	16	0.0915	0.4312	1.0847	2.4671	1.0852	0.0838	0.7788	4.3462	15.5846	44.6365
Cl	17	0.0799	0.3891	1.0037	2.3332	1.0507	0.0694	0.6443	3.5351	12.5058	35.8633
Ar	18	0.1044	0.4551	1.4232	2.1533	0.4459	0.0853	0.7701	4.4684	14.5864	41.2474
K	19	0.2149	0.8703	2.4999	2.3591	3.0318	0.1660	1.6906	8.7447	46.7825	165.6923
Ca	20	0.2355	0.9916	2.3959	3.7252	2.5647	0.1742	1.8329	8.8407	47.4583	134.9613
Sc	21	0.4636	2.0802	2.9003	1.4193	2.4323	0.3682	4.0312	22.6493	71.8200	103.3691
Ti	22	0.2123	0.8960	2.1765	3.0436	2.4439	0.1399	1.4568	6.7534	33.1168	101.8238
V	23	0.2369	1.0774	2.1894	3.0825	1.7190	0.1505	1.6392	7.5691	36.8741	107.8517
Cr	24	0.1970	0.8228	2.0200	2.1717	1.7516	0.1197	1.1985	5.4097	25.2361	94.4290
Mn	25	0.1943	0.8190	1.9296	2.4968	2.0625	0.1135	1.1313	5.0341	24.1798	80.5598
Fe	26	0.1929	0.8239	1.8689	2.3694	1.9060	0.1087	1.0806	4.7637	22.8500	76.7309
Co	27	0.2186	0.9861	1.8540	2.3258	1.4685	0.1182	1.2300	5.4177	25.7602	80.8542
Ni	28	0.2313	1.0657	1.8229	2.2609	1.1883	0.1210	1.2691	5.6870	27.0917	83.0285
Cu	29	0.3501	1.6558	1.9582	0.2134	1.4109	0.1867	1.9917	11.3396	53.2619	63.2520
Zn	30	0.1780	0.8096	1.6744	1.9499	1.4495	0.0876	0.8650	3.8612	18.8726	64.7016
Ga	31	0.2135	0.9768	1.6669	2.5662	1.6790	0.1020	1.0219	4.6275	22.8742	80.1535
Ge	32	0.2135	0.9761	1.6555	2.8938	1.6356	0.0989	0.9845	4.5527	21.5563	70.3903
As	33	0.2059	0.9518	1.6372	3.0490	1.4756	0.0926	0.9182	4.3291	19.2996	58.9329
Se	34	0.1574	0.7614	1.4834	3.0016	1.7978	0.0686	0.6808	3.1163	14.3458	44.0455
Br	35	0.1899	0.8983	1.6358	3.1845	1.1518	0.0810	0.7957	3.9054	15.7701	45.6124
Kr	36	0.1742	0.8447	1.5944	3.1507	1.1338	0.0723	0.7123	3.5192	13.7724	39.1148
Rb	37	0.3781	1.4904	3.5753	3.0031	3.3272	0.1557	1.5347	9.9947	51.4251	185.9828
Sr	38	0.3723	1.4598	3.5124	4.4612	3.3031	0.1480	1.4643	9.2320	49.8807	148.0937
Y	39	0.3234	1.2737	3.2115	4.0563	3.7962	0.1244	1.1948	7.2756	34.1430	111.2079
Zr	40	0.2997	1.1879	3.1075	3.9740	3.5769	0.1121	1.0638	6.3891	28.7081	97.4289
Nb	41	0.1680	0.9370	2.7300	3.8150	3.0053	0.0597	0.6524	4.4317	19.5540	85.5011
Mo	42	0.3069	1.1714	3.2293	3.4254	2.1224	0.1101	1.0222	5.9613	25.1965	93.5831
Tc	43	0.2928	1.1267	3.1675	3.6619	2.5942	0.1020	0.9481	5.4713	23.8153	82.8991
Ru	44	0.2604	1.0442	3.0761	3.2175	1.9448	0.0887	0.8240	4.8278	19.8977	80.4566
Rh	45	0.2713	1.0556	3.1416	3.0451	1.7179	0.0907	0.8324	4.7702	19.7862	80.2540
Pd	46	0.2003	0.8779	2.6135	2.8594	1.0258	0.0659	0.6111	3.5563	12.7638	44.4283
Ag	47	0.2739	1.0503	3.1564	2.7543	1.4328	0.0881	0.8028	4.4451	18.7011	79.2633
Cd	48	0.3072	1.1303	3.2046	2.9329	1.6560	0.0966	0.8856	4.6273	20.6789	73.4723
In	49	0.3564	1.3011	3.2424	3.4839	2.0459	0.1091	1.0452	5.0900	24.6578	88.0513
Sn	50	0.2966	1.1157	3.0973	3.8156	2.5281	0.0896	0.8268	4.2242	20.6900	71.3399
Sb	51	0.2725	1.0651	2.9940	4.0697	2.5682	0.0809	0.7488	3.8710	18.8800	60.6499
Te	52	0.2422	0.9692	2.8114	4.1509	2.8161	0.0708	0.6472	3.3609	16.0752	50.1724
I	53	0.2617	1.0325	2.8097	4.4809	2.3190	0.0749	0.6914	3.4634	16.3603	48.2522
Xe	54	0.2334	0.9496	2.6381	4.4680	2.5020	0.0655	0.6050	3.0389	14.0809	41.0005
Cs	55	0.5713	2.4866	4.9795	4.0198	4.4403	0.1626	1.8213	11.1049	49.0568	202.9987
Ba	56	0.5229	2.2874	4.7243	5.0807	5.6389	0.1434	1.6019	9.4511	42.7685	148.4969
La	57	0.5461	2.3856	5.0653	5.7601	4.0463	0.1479	1.6552	10.0059	47.3245	145.8464
Ce	58	0.2227	1.0760	2.9482	5.8496	7.1834	0.0571	0.5946	3.2022	16.4253	95.7030
Pr	59	0.5237	2.2913	4.6161	4.7233	4.8173	0.1360	1.5068	8.8213	41.9536	141.2424
Nd	60	0.5368	2.3301	4.6058	4.6621	4.4622	0.1378	1.5140	8.8719	43.5967	141.8065
Pm	61	0.5232	2.2627	4.4552	4.4787	4.5073	0.1317	1.4336	8.3087	40.6010	135.9196
Sm	62	0.5162	2.2302	4.3449	4.3598	4.4292	0.1279	1.3811	7.9629	39.1213	132.7846
Eu	63	0.5272	2.2844	4.3361	4.3178	4.0908	0.1285	1.3943	8.1081	40.9631	134.1233
Gd	64	0.9664	3.4052	5.0803	1.4991	4.2528	0.2641	2.6586	16.2213	80.2060	92.5359
Tb	65	0.5110	2.1570	4.0308	3.9936	4.2466	0.1210	1.2704	7.1368	35.0354	123.5062
Dy	66	0.4974	2.1097	3.8906	3.8100	4.3084	0.1157	1.2108	6.7377	32.4150	116.9225

Table 3. *(cont.)*

Element	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5
Ho	67	0.4679	1.9693	3.7191	3.9632	4.2432	0.1069	1.0994	5.9769	27.1491	96.3119
Er	68	0.5034	2.1088	3.8232	3.7299	3.8963	0.1141	1.1769	6.6087	33.4332	116.4913
Tm	69	0.4839	2.0262	3.6851	3.5874	4.0037	0.1081	1.1012	6.1114	30.3728	110.5988
Yb	70	0.5221	2.1695	3.7567	3.6685	3.4274	0.1148	1.1860	6.7520	35.6807	118.0692
Lu	71	0.4680	1.9466	3.5428	3.8490	3.6594	0.1015	1.0195	5.6058	27.4899	95.2846
Hf	72	0.4048	1.7370	3.3399	3.9448	3.7293	0.0868	0.8585	4.6378	21.6900	80.2408
Ta	73	0.3835	1.6747	3.2986	4.0462	3.4303	0.0810	0.8020	4.3545	19.9644	73.6337
W	74	0.3661	1.6191	3.2455	4.0856	3.2064	0.0761	0.7543	4.0952	18.2886	68.0967
Re	75	0.3933	1.6973	3.4202	4.1274	2.6158	0.0806	0.7972	4.4237	19.5692	68.7477
Os	76	0.3854	1.6555	3.4129	4.1111	2.4106	0.0787	0.7638	4.2441	18.3700	65.1071
Ir	77	0.3510	1.5620	3.2946	4.0615	2.4382	0.0706	0.6904	3.8266	16.0812	58.7638
Pt	78	0.3083	1.4158	2.9662	3.9349	2.1709	0.0609	0.5993	3.1921	12.5285	49.7675
Au	79	0.3055	1.3945	2.9617	3.8990	2.0026	0.0596	0.5827	3.1035	11.9693	47.9106
Hg	80	0.3593	1.5736	3.5237	3.8109	1.6953	0.0694	0.6758	3.8457	15.6203	56.6614
Tl	81	0.3511	1.5489	3.5676	4.0900	2.5251	0.0672	0.6522	3.7420	15.9791	65.1354
Pb	82	0.3540	1.5453	3.5975	4.3152	2.7743	0.0668	0.6465	3.6968	16.2056	61.4909
Bi	83	0.3530	1.5258	3.5815	4.5532	3.0714	0.0661	0.6324	3.5906	15.9962	57.5760
Po	84	0.3673	1.5772	3.7079	4.8582	2.8440	0.0678	0.6527	3.7396	17.0668	55.9789
At	85	0.3547	1.5206	3.5621	5.0184	3.0075	0.0649	0.6188	3.4696	15.6090	49.4818
Rn	86	0.4586	1.7781	3.9877	5.7273	1.5460	0.0831	0.7840	4.3599	20.0128	62.1535
Fr	87	0.8282	2.9941	5.6597	4.9292	4.2889	0.1515	1.6163	9.7752	42.8480	190.7366
Ra	88	1.4129	4.4269	7.0460	-1.0573	8.6430	0.2921	3.1381	19.6767	102.0436	113.9798
Ac	89	0.7169	2.5710	5.1791	6.3484	5.6474	0.1263	1.2900	7.3686	32.4490	118.0558
Th	90	0.6958	2.4936	5.1269	6.6988	5.0799	0.1211	1.2247	6.9398	30.0991	105.1960
Pa	91	1.2502	4.2284	7.0489	1.1390	5.8222	0.2415	2.6442	16.3313	73.5757	91.9401
U	92	0.6410	2.2643	4.8713	5.9287	5.3935	0.1097	1.0644	5.7907	25.0261	101.3899
Np	93	0.6938	2.4652	5.1227	5.5965	4.8543	0.1171	1.1757	6.4053	27.5217	103.0482
Pu	94	0.6902	2.4509	5.1284	5.0339	4.8575	0.1153	1.1545	6.2291	27.0741	111.3150
Am	95	0.7577	2.7264	5.4184	4.8198	4.1013	0.1257	1.3044	7.1035	32.4649	118.8647
Cm	96	0.7567	2.7565	5.4364	5.1918	3.5643	0.1239	1.2979	7.0798	32.7871	110.1512
Bk	97	0.7492	2.7267	5.3521	5.0369	3.5321	0.1217	1.2651	6.8101	31.6088	106.4853
Cf	98	0.8100	3.0001	5.4635	4.1756	3.5066	0.1310	1.4038	7.6057	34.0186	90.5226

in the BK results are purely due to the larger interval of the grid that they used in their data file compared with *International Tables for Crystallography*. Had they used the complete data set as listed in *International Tables for Crystallography*, the E factor would have been absolutely zero in both Tables 2 and 4.

The largest fitting error for the full range of s up to $6\,\text{Å}^{-1}$ occurs at $Z = 88$ for Ra; the E factor is 0.217 for this case. As an illustration, in Fig. 1 we have plotted both numerical and fitted $f(s)$ curves for Ra; it is seen that even for the worst case our analytical fitting is still reasonable, especially for small values of s.

The data file used in the program *ELAS*98 is compiled using the data contained in *International Tables for Crystallography*, Vol. C, Table 4.3.1.1 (Cowley, 1992). In this table, values of electron atomic scattering factors in Å are listed for all neutral atoms for s up to $2\,\text{Å}^{-1}$. For the range $2.0 < s < 6.0\,\text{Å}^{-1}$, the most recent Dirac–Fock calculations of X-ray scattering factors by Rez *et al.* (1994) were used. These results were converted into electron scattering factors using the Mott formula

$$f^{(e)}(s) = (me^2/2h^2)[Z - f^x(s)]/s^2 = 0.023\,933\,754[Z - f^x(s)]/s^2. \quad (13)$$

The reason that we did not use the more recent X-ray data for the range $s < 2.0\,\text{Å}^{-1}$ is that the Mott formula becomes less accurate for small values of s (Peng & Cowley, 1988). As an illustration, we present in Fig. 2 two curves of $f^{(e)}(s)$: one uses the data as given in *International Tables for Crystallography* and the other uses the X-ray scattering factor (Table 3 of Rez *et al.*, 1994) and the Mott formula. For large values of s, these two curves are seen to be indistinguishable, but for small values of s noticeable differences exist.

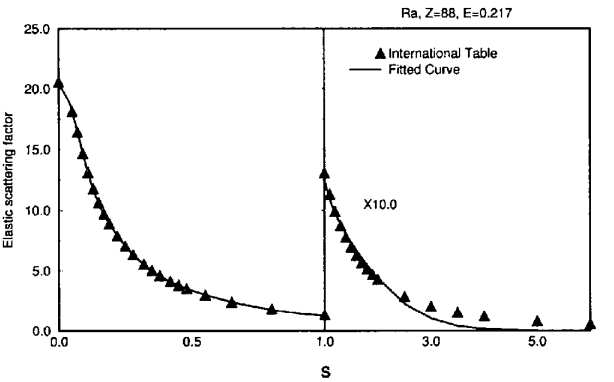


Fig. 1. Plot of elastic scattering factors for Ra as a function of s (Å^{-1}). The two curves shown in this figure are obtained using the data from *International Tables for Crystallography* and the analytical fitting parameters listed in Table 3.

Table 4. *Error analysis of Table 3*

In the table WK denotes Weickenmeier & Kohl (1991); DT denotes Doyle & Turner (1968), BK denotes Bird & King (1990) and PRDW denotes Peng, Ren, Dudarev & Whelan (this paper).

		WK		DT		BK		PRDW	
Element	Z	σ	E	σ	E	σ	E	σ	E
H	1					0.0015	0.2891	0.0011	0.2037
He	2	0.0083	1.9847	0.0007	0.1781	0.0003	0.0769	0.0003	0.0686
Li	3	0.0085	0.2599	0.0037	0.1138	0.0047	0.1432	0.0013	0.0392
Be	4	0.0078	0.2541	0.0029	0.0963	0.0011	0.0360	0.0009	0.0311
B	5	0.0132	0.4715	0.0029	0.1031	0.0007	0.0233	0.0009	0.0312
C	6	0.0110	0.4388	0.0029	0.1144	0.0004	0.0169	0.0009	0.0351
N	7	0.0039	0.1756	0.0032	0.1426	0.0013	0.0593	0.0014	0.0646
O	8	0.0157	0.7940	0.0029	0.1483	0.0003	0.0160	0.0006	0.0313
F	9	0.0022	0.1208	0.0031	0.1700	0.0003	0.0174	0.0006	0.0313
Ne	10	0.0027	0.1661	0.0032	0.1932	0.0003	0.0200	0.0005	0.0294
Na	11	0.0280	0.5859	0.0086	0.1808	0.0070	0.1460	0.0033	0.0680
Mg	12	0.0428	0.8222	0.0077	0.1470	0.0027	0.0514	0.0025	0.0481
Al	13	0.0551	0.9352	0.0087	0.1477	0.0025	0.0432	0.0030	0.0507
Si	14	0.0229	0.3921	0.0080	0.1376	0.0018	0.0301	0.0050	0.0862
P	15	0.0217	0.3955	0.0072	0.1320	0.0012	0.0214	0.0021	0.0387
S	16	0.0158	0.3064	0.0069	0.1330	0.0010	0.0193	0.0018	0.0349
Cl	17	0.0474	0.9767	0.0067	0.1380	0.0005	0.0111	0.0016	0.0320
Ar	18	0.0420	0.9179	0.0066	0.1446	0.0004	0.0090	0.0019	0.0411
K	19	0.0307	0.3413	0.0179	0.1995	0.0230	0.2560	0.0066	0.0730
Ca	20	0.0913	0.9215	0.0159	0.1600	0.0114	0.1147	0.0059	0.0593
Sc	21	0.0774	0.8312	0.0149	0.1606	0.0074	0.0800	0.0128	0.1375
Ti	22	0.0200	0.2275	0.0144	0.1644	0.0056	0.0639	0.0048	0.0552
V	23	0.0294	0.3538	0.0140	0.1686	0.0043	0.0521	0.0052	0.0628
Cr	24	0.0863	1.2378	0.0138	0.1975	0.0034	0.0484	0.0047	0.0678
Mn	25	0.0287	0.3829	0.0135	0.1795	0.0028	0.0379	0.0044	0.0584
Fe	26	0.0314	0.4388	0.0133	0.1861	0.0023	0.0326	0.0043	0.0594
Co	27	0.0576	0.8404	0.0132	0.1927	0.0020	0.0292	0.0042	0.0610
Ni	28	0.0420	0.6399	0.0131	0.1998	0.0017	0.0259	0.0044	0.0668
Cu	29	0.0682	1.2182	0.0132	0.2350	0.0014	0.0255	0.0107	0.1903
Zn	30	0.0463	0.7631	0.0131	0.2152	0.0013	0.0210	0.0036	0.0595
Ga	31	0.0484	0.6811	0.0154	0.2167	0.0024	0.0332	0.0049	0.0687
Ge	32	0.0778	1.0540	0.0148	0.2000	0.0018	0.0239	0.0043	0.0581
As	33	0.0454	0.6198	0.0139	0.1895	0.0013	0.0177	0.0038	0.0516
Se	34	0.0130	0.1801	0.0133	0.1849	0.0012	0.0173	0.0032	0.0445
Br	35	0.0262	0.3711	0.0131	0.1849	0.0011	0.0150	0.0033	0.0467
Kr	36	0.0254	0.3688	0.0129	0.1869	0.0007	0.0108	0.0029	0.0418
Rb	37	0.1035	0.8789	0.0288	0.2442	0.0311	0.2640	0.0101	0.0860
Sr	38	0.0554	0.4229	0.0272	0.2074	0.0180	0.1376	0.0096	0.0729
Y	39	0.1148	0.9057			0.0092	0.0724	0.0082	0.0644
Zr	40	0.0876	0.7196			0.0063	0.0518	0.0080	0.0655
Nb	41	0.0929	0.8703			0.0426	0.3990	0.0096	0.0901
Mo	42	0.0858	0.8363	0.0217	0.2115	0.0040	0.0388	0.0068	0.0659
Tc	43	0.0698	0.6427			0.0029	0.0265	0.0069	0.0634
Ru	44	0.0807	0.8445			0.0024	0.0248	0.0064	0.0675
Rh	45	0.0795	0.8605			0.0020	0.0221	0.0061	0.0663
Pd	46	0.0427	0.5625			0.0018	0.0237	0.0039	0.0509
Ag	47	0.0961	1.1082	0.0200	0.2302	0.0019	0.0217	0.0059	0.0680
Cd	48	0.0521	0.5640	0.0199	0.2152	0.0017	0.0188	0.0060	0.0655
In	49	0.0920	0.8822	0.0227	0.2174	0.0033	0.0314	0.0075	0.0716
Sn	50	0.1082	0.9962	0.0219	0.2015	0.0026	0.0243	0.0068	0.0630
Sb	51	0.0614	0.5598	0.0208	0.1896	0.0022	0.0203	0.0060	0.0544
Te	52	0.0258	0.2343			0.0023	0.0214	0.0055	0.0496
I	53	0.0668	0.6130	0.0195	0.1788	0.0019	0.0174	0.0050	0.0462
Xe	54	0.0321	0.2978	0.0190	0.1760	0.0015	0.0143	0.0044	0.0404
Cs	55	0.1684	1.0204	0.0410	0.2482	0.0488	0.2957	0.0148	0.0895
Ba	56	0.0657	0.3598	0.0404	0.2210	0.0330	0.1806	0.0132	0.0725
La	57	0.0922	0.5180			0.0166	0.0931	0.0133	0.0745
Ce	58	0.0925	0.5326			0.0142	0.0819	0.0308	0.1772
Pr	59	0.0760	0.4476			0.0167	0.0986	0.0127	0.0750
Nd	60	0.0791	0.4762			0.0173	0.1043	0.0125	0.0751
Pm	61	0.0793	0.4879			0.0150	0.0924	0.0122	0.0753
Sm	62	0.0764	0.4807			0.0151	0.0947	0.0122	0.0769
Eu	63	0.1190	0.7647	1.3211	8.4887	0.0184	0.1183	0.0118	0.0757

Table 4. *(cont.)*

		WK		DT		BK		PRDW	
Element	Z	σ	E	σ	E	σ	E	σ	E
Gd	64	0.0550	0.3603			0.0111	0.0726	0.0321	0.2100
Tb	65	0.0950	0.6346			0.0113	0.0755	0.0130	0.0865
Dy	66	0.0879	0.6004			0.0121	0.0825	0.0120	0.0817
Ho	67	0.0403	0.2804			0.0082	0.0569	0.0101	0.0704
Er	68	0.0994	0.7057			0.0116	0.0824	0.0114	0.0806
Tm	69	0.0413	0.2993			0.0090	0.0650	0.0115	0.0833
Yb	70	0.0451	0.3326			0.0094	0.0696	0.0111	0.0821
Lu	71	0.0402	0.2977			0.0071	0.0524	0.0102	0.0758
Hf	72	0.0442	0.3358			0.0069	0.0522	0.0099	0.0753
Ta	73	0.1293	1.0058			0.0042	0.0325	0.0094	0.0729
W	74	0.0543	0.4330			0.0027	0.0216	0.0091	0.0722
Re	75	0.1215	0.9906			0.0023	0.0185	0.0078	0.0634
Os	76	0.0817	0.6814			0.0037	0.0307	0.0076	0.0633
Ir	77	0.0939	0.8015			0.0022	0.0189	0.0070	0.0596
Pt	78	0.0729	0.6743			0.0023	0.0216	0.0075	0.0695
Au	79	0.0600	0.5673	0.0287	0.2710	0.0012	0.0110	0.0068	0.0641
Hg	80	0.0644	0.5874	0.0289	0.2640	0.0013	0.0122	0.0063	0.0571
Tl	81	0.1030	0.8506			0.0033	0.0269	0.0090	0.0743
Pb	82	0.0630	0.5002	0.0321	0.2547	0.0026	0.0208	0.0084	0.0664
Bi	83	0.0973	0.7430	0.0319	0.2439	0.0025	0.0188	0.0082	0.0626
Po	84	0.0572	0.4281			0.0026	0.0197	0.0073	0.0547
At	85	0.0503	0.3732			0.0024	0.0181	0.0066	0.0492
Rn	86	0.0436	0.3233	0.2074	1.5375	0.0021	0.0155	0.0095	0.0706
Fr	87	0.1552	0.8291			0.0266	0.1419	0.0204	0.1092
Ra	88	0.1593	0.7750			0.0215	0.1045	0.0446	0.2170
Ac	89	0.1077	0.5256			0.0159	0.0777	0.0167	0.0815
Th	90	0.1306	0.6495			0.0106	0.0529	0.0156	0.0776
Pa	91	0.1026	0.5242			0.0110	0.0561	0.0398	0.2033
U	92	0.1657	0.8667	0.0446	0.2335	0.0134	0.0700	0.0160	0.0835
Np	93	0.1082	0.5766			0.0115	0.0612	0.0158	0.0842
Pu	94	0.1378	0.7577			0.0120	0.0662	0.0159	0.0874
Am	95	0.1295	0.7262			0.0125	0.0698	0.0161	0.0900
Cm	96	0.1933	1.0913			0.0081	0.0460	0.0156	0.0879
Bk	97	0.1562	0.8972			0.0064	0.0370	0.0152	0.0874
Cf	98	0.1665	0.9884			0.0121	0.0717	0.0276	0.1638

We noted that Table 2 of Rez *et al.* (1994) is not complete. The neutral elements they omitted to consider were those with atomic numbers $Z = 1$, 43, 61 and 93–98. For elements with $Z > 1$, the data given in Table 1 of Fox *et al.* (1989) were used.

The second program that we developed in this study (*ABSOR98*) reads in the atomic number of the neutral atom for which the parameters are to be determined, the Debye–Waller factor at the corresponding temperature and the acceleration voltage and returns the fitting parameters together with the σ and E values. This program first calculates the absorptive scattering factors and then fits these factors using the routine *MCFIT*.

The numerical values of the absorptive structure factors are calculated based on the original formula of Hall & Hirsch (Hall & Hirsch, 1965; Bird & King, 1990):

$$f^{(e)}_{\rm abs}(s,M) = (2h/\beta m_0 c)\int {\rm d}\mathbf{s}' f^{(e)}(|(\mathbf{s}/2)+\mathbf{s}'|) \times f^{(e)}(|(\mathbf{s}/2)-\mathbf{s}'|) \times \{1-\exp[-2B(s'^2 - s^2/4)]\}, \quad (14)$$

where β is the velocity ratio $\beta = v/c$ and B (in Å^2) is the Debye–Waller factor (sometimes called the temperature factor), which is related to the mean square thermal vibration amplitude $\overline{u^2}$

$$B = 8\pi^2\overline{u^2}. \quad (15)$$

To calculate absorptive scattering factors accurately (see below), it is necessary to extend the elastic scattering factors out to s values of about 30 Å^{-1} (Bird & King, 1990). To add the tails of the scattering factors, for hydrogen at $s \geq 1.5$ Å^{-1} and all other elements at $s \geq 6.0$ Å^{-1}, a screened Coulomb potential is assumed and the asymptotic behaviour of the scattering amplitude of the Lorentzian form is used:

$$f(s) \rightarrow 0.023\,933\,754[{\rm Z}/(s^2+\alpha^2)], \quad (16)$$

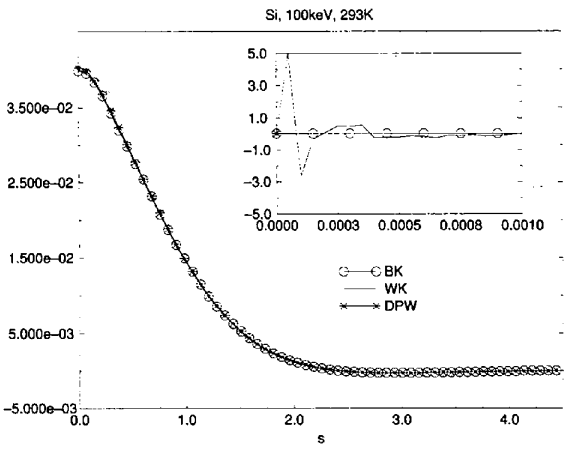
where α is related to the screening length of the screened Coulomb potential. In our program, α is determined simply by matching the numerical value of $f(s)$ at $s = 1.5$ Å^{-1} for hydrogen and at $s = 6.0$ Å^{-1} for all other elements to the limiting form (16).

There exist at least three sets of computer routines that can be obtained free of charge *via* electronic mail for

calculating absorptive scattering factors (Bird & King, 1990; Weickenmeier & Kohl, 1991; Dudarev *et al.*, 1995). Currently, the most quoted routine is perhaps the first one by Bird & King (1990). This routine is basically a data base that interpolates and returns both the elastic and absorptive scattering factors for $B < 2.0\,\text{Å}^2$ and $Bs^2 < 6.0$, where B is the Debye–Waller factor. For a typical element, such as an Si atom, the Debye–Waller factor is about $0.3\,\text{Å}^2$ at room temperature. This gives an upper limit of about $4\,\text{Å}^{-1}$ for s. There exist many other elements, such as Li, Na, Mg, K, Ca, Rd, Sr, Cd, Cs, Ba, La, Ce and Ti, that have Debye–Waller factors greater than $1\,\text{Å}^2$ at room temperature. This routine is therefore not applicable for large values of s and large B values. The alternative routine given by Weickenmeier & Kohl (1991) is not subjected to small or intermediate values of s but results as calculated from this routine suffer from an instability for very small values of s. Shown in Fig. 3 is an example of the $f_{\text{abs}}^{(e)}(s)$ curves calculated using the three routines. The computation has been made for 100 keV incident electrons and for an Si atom. It is seen that, while results calculated using all the three routines agree well with each other for most s values, the routine given by Weickenmeier & Kohl (1991) produces an artificial oscillation for very small values of s (see the insert of Fig. 3*a*) and the routine by Bird & King returns zero for all values of $s > 4\,\text{Å}^{-1}$ (see Fig. 3*b*). Although the routine by Dudarev *et al.* (1995) works well for all values of s, this routine is slower than the other two routines. In the present work, we have incorporated the routine of Bird & King for small values of s, and that by Weickenmeier & Kohl for intermediate and large values of s for calculating the absorptive scattering factors for all neutral atoms.

Listed in Tables 5 to 21 are parameterizations of the electron absorptive scattering factors over the range of s up to $6.0\,\text{Å}^{-1}$ for 17 important materials with the zinc blende structure over the temperature range 70 to 295 K.* These materials are GaP, GaSb, GaAs, InP, InSb, InAs, ZnO, ZnS, ZnSe, ZnTe, CdTe, HgSe, HgTe, CuCl, CuBr, CuI and SiC. Debye–Waller factors for these materials were taken from Reid (1983), which are calculated using a shell model and show very good correlation with experimental measurements. All results shown in Tables 5 to 21 were calculated for 100 keV incident electrons. The fitted numerical quantities are indeed $f_{\text{abs}}^{(e)}(s)\exp[-(1/2)Bs^2]$, rather than the absorptive scattering factors. This is because the absorptive scattering factors increase with s as $\exp[(1/2)Bs^2]$ at

* More extensive tables giving electronic absorptive scattering factors for the temperature range 1 to 1000 K have been deposited with the IUCr (Reference: ZH0006). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.



(*a*)

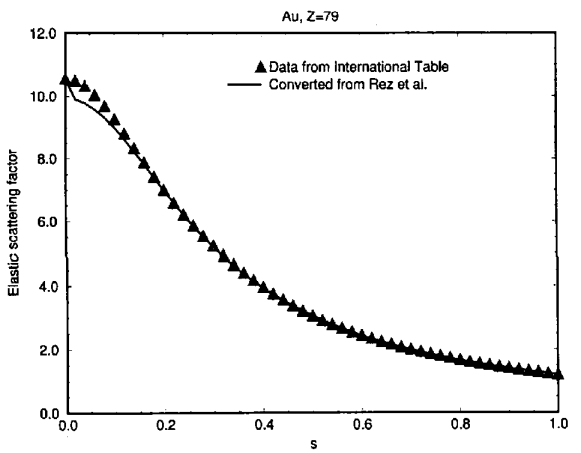
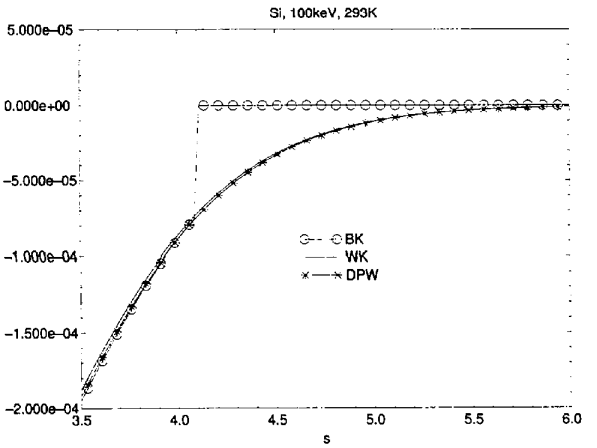


Fig. 2. Plot of elastic scattering factors for Au. The two curves in the figure are obtained from the data listed in *International Tables for Crystallography* and that converted from the X-ray scattering factors of Rez *et al.* using the Mott formula.



(*b*)

Fig. 3. Plot of absorptive scattering factors for the range (*a*) $s = 0 \rightarrow 4.5\,\text{Å}^{-1}$ and (*b*) $s = 3.5 \rightarrow 6.0\,\text{Å}^{-1}$. The three curves are obtained using the computer routines by BK, WK and DPW.

Table 5. *Absorptive scattering factors for GaP and s up to 6.0 Å^{-1}*

(*a*) Ga

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.1699	−0.0110	0.0479	0.0331	0.0261	0.0065	0.0309	0.1514	0.4278	1.1970	3.8907	0.5682E−04
80.0	0.1819	−0.0087	0.0602	0.0421	0.0228	−0.0094	0.0253	0.1918	0.7572	2.9851	3.1934	0.6545E−04
90.0	0.1946	−0.0113	0.0562	0.0387	0.0240	0.0041	0.0331	0.1807	0.5536	1.5548	5.3501	0.4523E−04
100.0	0.2080	−0.0118	0.0600	0.0418	0.0229	0.0036	0.0351	0.1942	0.6089	1.7239	5.9474	0.3931E−04
150.0	0.2802	−0.0137	0.0836	0.0579	0.0121	−0.0004	0.0441	0.2767	1.0261	4.2487	11.9690	0.6040E−04
200.0	0.3576	−0.0162	0.1044	0.0656	0.0114	−0.0049	0.0550	0.3564	1.3337	9.4981	18.5515	0.9193E−04
250.0	0.4373	−0.0193	0.1156	0.0698	0.0132	0.0006	0.0674	0.4163	1.3176	4.4502	20.2167	0.5414E−04
295.0	0.5101	−0.0208	0.1373	0.0725	0.0074	−0.0004	0.0758	0.4985	1.6860	9.7140	25.4229	0.8834E−04

(*b*) P

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2421	−0.0031	0.0196	0.0137	0.0047	0.0009	0.0383	0.2499	1.0121	5.2097	64.0090	0.2145E−04
80.0	0.2554	−0.0033	0.0202	0.0143	0.0050	0.0010	0.0412	0.2589	1.0214	5.1757	69.0532	0.2274E−04
90.0	0.2695	−0.0035	0.0209	0.0148	0.0052	0.0010	0.0437	0.2702	1.0433	5.2748	71.5722	0.2335E−04
100.0	0.2843	−0.0031	0.0246	0.0149	0.0034	−0.0003	0.0394	0.3211	1.5751	17.7587	66.4423	0.6340E−04
150.0	0.3657	−0.0041	0.0286	0.0174	0.0042	0.0001	0.0552	0.3830	1.6325	13.0120	55.9706	0.4440E−04
200.0	0.4546	−0.0049	0.0330	0.0191	0.0049	0.0006	0.0687	0.4600	1.7684	11.1218	50.6624	0.3404E−04
250.0	0.5478	−0.0054	0.0399	0.0197	0.0050	−0.0005	0.0786	0.5702	2.3609	20.9908	51.7633	0.6252E−04
295.0	0.6339	−0.0059	0.0452	0.0202	0.0096	−0.0053	0.0889	0.6599	2.7739	30.4735	41.1332	0.7163E−04

Table 6. *Absorptive scattering factors for GaSb and s up to 6.0 Å^{-1}*

(*a*) Ga

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2706	−0.0147	0.0734	0.0539	0.0228	0.0012	0.0458	0.2472	0.7703	2.3960	16.9936	0.3783E−04
80.0	0.2961	−0.0147	0.0852	0.0593	0.0142	−0.0001	0.0474	0.2859	1.0022	3.7018	30.8371	0.5682E−04
90.0	0.3225	−0.0149	0.0958	0.0624	0.0091	−0.0013	0.0496	0.3230	1.2207	6.4484	32.9944	0.8453E−04
100.0	0.3496	−0.0172	0.0919	0.0640	0.0194	0.0000	0.0566	0.3230	0.9987	3.2497	39.0313	0.6485E−04
150.0	0.4911	−0.0209	0.1222	0.0683	0.0210	0.0014	0.0747	0.4586	1.2753	3.4921	38.4235	0.8004E−04
200.0	0.6382	−0.0241	0.1588	0.0694	0.0146	0.0021	0.0921	0.6091	1.7406	4.4582	36.3243	0.1413E−03
250.0	0.7878	−0.0272	0.1928	0.0696	0.0082	0.0014	0.1094	0.7550	2.2521	6.8065	35.2097	0.2108E−03
295.0	0.9237	−0.0014	−0.0339	0.2181	0.0779	0.0039	0.0152	0.1556	0.8369	2.6844	31.6069	0.1061E−03

(*b*) Sb

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2192	−0.0206	0.2084	0.0960	0.0545	−0.0462	0.0234	0.2601	1.4029	33.1165	40.8234	0.5384E−03
80.0	0.2422	−0.0238	0.2233	0.1021	0.0527	−0.0441	0.0287	0.2787	1.4750	35.3758	43.9657	0.5500E−03
90.0	0.2659	−0.0275	0.2370	0.1085	0.0323	−0.0228	0.0346	0.2959	1.5131	29.8965	44.8214	0.5279E−03
100.0	0.2900	−0.0307	0.2508	0.1140	0.0272	−0.0172	0.0397	0.3143	1.5633	25.5476	43.2299	0.4937E−03
150.0	0.4149	−0.0441	0.3106	0.1378	0.0216	−0.0056	0.0610	0.4086	1.7408	13.7343	41.4639	0.3094E−03
200.0	0.5434	−0.0524	0.3696	0.1514	0.0201	−0.0017	0.0771	0.5168	2.0706	13.8029	37.8739	0.3001E−03
250.0	0.6735	−0.0588	0.4240	0.1586	0.0200	−0.0012	0.0916	0.6275	2.3964	13.1473	38.4018	0.3712E−03
295.0	0.7912	−0.0641	0.4649	0.1599	0.0246	0.0021	0.1045	0.7221	2.5398	8.9457	36.8746	0.4874E−03

large angles of scattering, while the quantity that we fitted, $f_{\rm abs}^{(e)}(s)\exp(-Bs^2/2.0)$, vanishes with increasing s (Dudarev *et al.*, 1995). In general, the crystal structure factor V_g is given by

$$V_g = (\hbar^2/2m_0)(4\pi/\Omega)\sum_n \exp(-i\mathbf{g}\cdot\mathbf{r}_n) \times \sum_{i=1}^{5}\left\{a_{i,n}^{\rm (Re)}\exp[-(b_{i,n}^{\rm (Re)}+B_n)s^2] + ia_{i,n}^{\rm (Im)}\exp[-(b_{i,n}^{\rm (Im)}+B_n/2)s^2]\right\}, \quad (17)$$

in which $g = 4\pi s$, n labels the atoms within a unit cell with position vector $\mathbf{r}_n$, Ω is the unit-cell volume and the superscripts Re and Im refer to the real and imaginary coefficients listed in Tables 2, 4 (real) and 5–21 (imaginary), respectively. Although (14) shows that the absorptive scattering factors depend on the acceleration voltage, results for any other acceleration voltage E can be converted *via* the following relations:

$$f_{\rm abs}^{(e)}(s,E) = [\beta(100\,{\rm keV})/\beta(E)]f_{\rm abs}^{(e)}(s,100\,{\rm keV}), \quad (18)$$

where $\beta = (1-\gamma^{-2})^{1/2}$, $\gamma = (m/m_0) = 1.0 + 1.956\,934\,1\times10^{-3}E$, and the acceleration voltage E is in keV.

Table 7. *Absorptive scattering factors for GaAs and s up to 6.0 Å^{-1}*

(*a*) Ga

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2008	−0.0133	0.0477	0.0366	0.0337	0.0093	0.0377	0.1643	0.3914	1.0820	3.6230	0.4596E−04
80.0	0.2171	−0.0131	0.0560	0.0378	0.0313	0.0076	0.0386	0.1889	0.4885	1.2676	4.2413	0.3833E−04
90.0	0.2341	−0.0133	0.0637	0.0444	0.0263	0.0042	0.0401	0.2121	0.6213	1.6967	6.1910	0.2990E−04
100.0	0.2516	−0.0147	0.0594	0.0392	0.0375	0.0095	0.0443	0.2135	0.4919	1.2271	4.1300	0.3525E−04
150.0	0.3452	−0.0171	0.0883	0.0563	0.0247	0.0050	0.0563	0.3146	0.8854	2.1171	5.8277	0.5777E−04
200.0	0.4439	−0.0193	0.1202	0.1143	−0.0865	0.0526	0.0679	0.4281	1.6152	2.4452	3.4495	0.6672E−04
250.0	0.5451	−0.0009	−0.0260	0.1300	0.0847	0.0151	0.0024	0.1021	0.4738	1.3920	5.4371	0.7352E−04
295.0	0.6373	−0.0239	0.1607	0.0616	0.0184	0.0038	0.0915	0.6132	1.7431	3.2743	18.9174	0.1401E−03

(*b*) As

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2095	−0.0132	0.0669	0.0485	0.0242	0.0044	0.0352	0.1952	0.6181	1.7736	7.4795	0.3116E−04
80.0	0.2276	−0.0153	0.0623	0.0439	0.0374	0.0094	0.0407	0.1938	0.4815	1.2276	4.8249	0.3314E−04
90.0	0.2464	−0.0154	0.0729	0.0524	0.0285	0.0060	0.0422	0.2212	0.6394	1.6906	6.7065	0.3044E−04
100.0	0.2657	−0.0167	0.0711	0.0466	0.0399	0.0101	0.0459	0.2291	0.5498	1.3107	5.0224	0.4233E−04
150.0	0.3682	−0.0189	−0.0081	0.1144	0.0760	0.0187	0.0579	0.2231	0.3328	1.0601	4.0395	0.1177E−03
200.0	0.4757	−0.0224	0.1434	0.1260	−0.2815	0.2447	0.0721	0.4618	1.7200	2.9774	3.3031	0.1260E−03
250.0	0.5855	−0.0015	−0.0308	0.1503	0.0957	0.0212	0.0118	0.1128	0.5000	1.3704	5.1922	0.1105E−03
295.0	0.6853	−0.0011	−0.0330	0.1803	0.0915	0.0166	0.0045	0.1227	0.6050	1.7058	6.2658	0.1860E−03

Table 8. *Absorptive scattering factors for InP and s up to 6.0 Å^{-1}*

(*a*) In

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2438	−0.0335	0.1318	0.0922	0.0707	0.0275	0.0425	0.1994	0.4498	1.1422	4.2506	0.1280E−03
80.0	0.2694	−0.0331	0.1717	0.1143	0.0475	0.0059	0.0440	0.2421	0.7280	2.5747	10.8126	0.1059E−03
90.0	0.2957	−0.0353	0.1859	0.1199	0.0480	0.0043	0.0480	0.2659	0.7962	2.8609	11.8005	0.1179E−03
100.0	0.3226	−0.0344	0.2222	0.1236	0.2201	−0.1927	0.0489	0.3129	1.1413	7.6510	8.1186	0.1872E−03
150.0	0.4622	−0.0452	0.2714	0.1109	0.0579	0.0195	0.0690	0.4225	1.1091	2.4775	7.5598	0.1305E−03
200.0	0.6057	−0.0016	−0.0562	0.3585	0.1531	0.0248	0.0006	0.1000	0.5514	1.9434	9.4064	0.2029E−03
250.0	0.7509	−0.0019	−0.0649	0.4191	0.1611	0.0189	0.0004	0.1223	0.6704	2.3988	12.1256	0.1753E−03
295.0	0.8824	−0.0045	−0.0737	0.4569	0.1740	0.0233	0.0228	0.1532	0.7540	2.5195	11.7658	0.1595E−03

(*b*) P

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2268	−0.0019	0.0222	0.0124	0.0138	−0.0124	0.0203	0.2950	1.8326	119.3996	141.8956	0.1161E−03
80.0	0.2391	−0.0021	0.0231	0.0128	0.0168	−0.0153	0.0233	0.3065	1.8783	121.5964	140.4974	0.1182E−03
90.0	0.2519	−0.0022	0.0241	0.0132	0.0133	−0.0117	0.0267	0.3188	1.9309	122.6450	148.4962	0.1207E−03
100.0	0.2652	−0.0024	0.0250	0.0136	0.0131	−0.0114	0.0291	0.3320	1.9752	119.3160	146.0495	0.1217E−03
150.0	0.3376	−0.0032	0.0299	0.0155	0.0148	−0.0130	0.0437	0.4010	2.2582	120.6112	147.0249	0.1274E−03
200.0	0.4171	−0.0039	0.0350	0.0169	0.0184	−0.0164	0.0558	0.4800	2.6046	121.2542	142.4344	0.1277E−03
250.0	0.5008	−0.0046	0.0403	0.0179	0.0205	−0.0184	0.0677	0.5656	3.0020	123.0362	142.3330	0.1252E−03
295.0	0.5783	−0.0051	0.0449	0.0186	0.0158	−0.0135	0.0773	0.6438	3.3718	121.1568	147.0295	0.1219E−03

Table 9. *Absorptive scattering factors for InSb and s up to 6.0 Å^{-1}*

(*a*) In

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.3547	−0.0374	0.2349	0.1282	0.0389	−0.0072	0.0542	0.3375	1.1674	5.6887	11.1251	0.1531E−03
80.0	0.3962	−0.0419	0.2370	0.1300	0.0523	0.0032	0.0613	0.3582	1.0208	3.4514	17.3056	0.1119E−03
90.0	0.4385	−0.0437	0.2667	0.1325	0.0449	0.0024	0.0661	0.4046	1.2234	4.2144	21.4898	0.1030E−03
100.0	0.4814	−0.0465	0.2801	0.1291	0.0567	0.0048	0.0717	0.4385	1.2066	3.6670	24.4580	0.1483E−03
150.0	0.7004	−0.0016	−0.0590	0.4139	0.1511	0.0101	0.0007	0.1100	0.6521	2.6191	23.3590	0.3168E−03
200.0	0.9233	−0.0025	−0.0722	0.4881	0.1646	0.0113	0.0086	0.1466	0.8164	3.0759	28.0019	0.2482E−03
250.0	1.1479	−0.0062	−0.0832	0.5516	0.1773	0.0125	0.0364	0.1934	0.9681	3.4451	31.1201	0.2126E−03
295.0	1.3508	−0.0777	0.6246	0.1567	−0.0131	0.0091	0.1638	1.2017	4.7661	8.4009	40.3508	0.8761E−03

Table 9 (*cont.*)

(*b*) Sb

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2997	−0.0316	0.2576	0.1156	0.0456	−0.0370	0.0412	0.3239	1.6264	34.9312	46.3941	0.5286E−03
80.0	0.3341	−0.0358	0.2743	0.1231	0.0201	−0.0095	0.0476	0.3488	1.6533	20.9628	53.9854	0.4476E−03
90.0	0.3692	−0.0388	0.2940	0.1285	0.0221	−0.0121	0.0529	0.3796	1.7764	24.9457	54.7160	0.4487E−03
100.0	0.4047	−0.0435	0.3038	0.1366	0.0211	−0.0033	0.0597	0.3982	1.6714	11.2997	49.9679	0.2837E−03
150.0	0.5868	−0.0561	0.3705	0.1432	0.0445	0.0051	0.0834	0.5372	1.7258	5.0672	42.8072	0.2683E−03
200.0	0.7724	−0.0630	0.4607	0.1603	0.0216	0.0007	0.1022	0.7096	2.5777	10.4891	39.3313	0.4668E−03
250.0	0.9597	−0.0695	0.5344	0.0922	0.0794	0.0089	0.1211	0.8735	2.8222	4.2151	40.2742	0.6722E−03
295.0	1.1289	−0.0058	−0.0861	0.5832	0.1919	0.0127	0.0316	0.1834	0.9539	3.4845	35.5217	0.2823E−03

Table 10. *Absorptive scattering factors for ZnO and s up to 6.0 Å^{-1}*

(*a*) Zn

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.1816	−0.0097	0.0512	0.0361	0.0212	0.0024	0.0301	0.1740	0.5735	1.6968	7.2246	0.3489E−04
80.0	0.1937	−0.0116	0.0467	0.0327	0.0300	0.0075	0.0354	0.1665	0.4285	1.1546	3.8845	0.3913E−04
90.0	0.2068	−0.0121	0.0499	0.0355	0.0299	0.0066	0.0375	0.1787	0.4726	1.2670	4.3769	0.3821E−04
100.0	0.2205	−0.0123	0.0541	0.0372	0.0294	0.0059	0.0391	0.1944	0.5287	1.3764	4.9344	0.3834E−04
150.0	0.2958	−0.0147	0.0705	0.0469	0.0283	0.0054	0.0500	0.2656	0.7291	1.7339	5.7131	0.2091E−04
200.0	0.3769	−0.0167	0.0922	0.0619	0.0174	0.0019	0.0602	0.3530	1.0760	2.9567	9.4635	0.3084E−04
250.0	0.4607	−0.0188	0.1107	0.0638	0.0158	0.0041	0.0710	0.4368	1.2802	2.8448	8.8555	0.5358E−04
295.0	0.5374	−0.0205	0.1282	0.0375	0.0397	0.0060	0.0803	0.5165	1.3168	2.0304	9.2903	0.9089E−04

(*b*) O

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2411	−0.0010	0.0054	0.0039	0.0027	0.0007	0.0408	0.2471	0.8738	2.7514	6.5825	0.3025E−05
80.0	0.2479	−0.0009	0.0061	0.0046	0.0024	−0.0002	0.0383	0.2751	1.2158	4.8303	7.8895	0.7264E−05
90.0	0.2551	−0.0011	0.0056	0.0039	0.0031	0.0007	0.0442	0.2553	0.8545	2.6510	7.2470	0.2091E−05
100.0	0.2627	−0.0011	0.0057	0.0041	0.0034	0.0004	0.0457	0.2604	0.8714	2.8841	10.2711	0.1959E−05
150.0	0.3054	−0.0012	0.0068	0.0052	−0.0083	0.0112	0.0511	0.3144	1.2128	3.5885	3.7490	0.4812E−05
200.0	0.3546	−0.0014	0.0068	0.0037	0.0041	0.0020	0.0608	0.3377	0.8765	2.0368	5.1948	0.2408E−05
250.0	0.4085	−0.0014	0.0090	0.0071	0.0027	−0.0007	0.0656	0.4277	1.7622	7.0469	11.9002	0.6958E−05
295.0	0.4600	−0.0016	0.0093	0.0067	0.0034	0.0001	0.0742	0.4620	1.5949	4.4807	19.1554	0.4781E−05

Table 11. *Absorptive scattering factors for InAs and s up to 6.0 Å^{-1}*

(*a*) In

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2585	−0.0264	0.1970	0.1092	0.0302	−0.0113	0.0359	0.2691	1.1258	8.5562	16.0069	0.2913E−03
80.0	0.2864	−0.0349	0.1790	0.1201	0.0494	0.0036	0.0470	0.2551	0.7602	2.8333	15.2361	0.1184E−03
90.0	0.3150	−0.0349	0.2101	0.1224	0.0375	−0.0008	0.0489	0.2975	1.0013	4.2594	13.6450	0.1400E−03
100.0	0.3441	−0.0380	0.2177	0.1267	0.0441	0.0009	0.0539	0.3164	0.9834	3.7460	17.8278	0.1227E−03
150.0	0.4945	−0.0470	0.2848	0.1206	0.0631	0.0088	0.0730	0.4506	1.1799	3.1706	14.6049	0.1635E−03
200.0	0.6489	−0.0535	0.3676	0.0814	0.0884	0.0118	0.0899	0.6026	1.4995	3.0377	16.2850	0.3303E−03
250.0	0.8049	−0.0050	−0.0714	0.4205	0.1734	0.0330	0.0243	0.1457	0.6812	2.1409	8.3632	0.1292E−03
295.0	0.9461	−0.0055	−0.0766	0.4787	0.1773	0.0218	0.0297	0.1657	0.8015	2.6835	13.3684	0.1783E−03

(*b*) As

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.1983	−0.0124	0.0652	0.0475	0.0225	0.0037	0.0329	0.1879	0.6183	1.8441	7.9855	0.3455E−04
80.0	0.2151	−0.0139	0.0654	0.0456	0.0290	0.0069	0.0371	0.1942	0.5597	1.4546	5.6179	0.2869E−04
90.0	0.2326	−0.0143	0.0719	0.0494	0.0252	0.0073	0.0391	0.2145	0.6467	1.5999	5.5437	0.3125E−04
100.0	0.2506	−0.0157	0.0734	0.0524	0.0292	0.0067	0.0431	0.2237	0.6363	1.6451	6.2516	0.3109E−04
150.0	0.3458	−0.0188	0.1021	0.0674	0.0096	0.0155	0.0560	0.3218	0.9785	1.8029	4.2048	0.1104E−03
200.0	0.4458	−0.0009	−0.0245	0.1241	0.0846	0.0194	0.0025	0.0832	0.3958	1.1804	4.5368	0.1123E−03
250.0	0.5481	−0.0008	−0.0278	0.1518	0.0880	0.0158	0.0007	0.0983	0.4941	1.4736	6.0578	0.1088E−03
295.0	0.6412	−0.0272	0.1767	0.0782	0.0193	−0.0013	0.0928	0.6094	1.6910	6.0243	21.9383	0.2021E−03

Table 12. *Absorptive scattering factors for ZnS and s up to 6.0 Å^{-1}*

(*a*) Zn

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2582	−0.0113	0.0760	0.0535	0.0085	−0.0009	0.0385	0.2679	1.0896	5.9105	13.9498	0.8709E−04
80.0	0.2807	−0.0142	0.0668	0.0450	0.0298	0.0049	0.0476	0.2510	0.6805	1.6818	6.2613	0.2658E−04
90.0	0.3042	−0.0142	0.0798	0.0570	0.0146	0.0012	0.0491	0.2911	0.9861	3.1123	9.8026	0.3047E−04
100.0	0.3285	−0.0156	0.0792	0.0556	0.0236	0.0021	0.0542	0.3001	0.8771	2.3576	10.0044	0.2411E−04
150.0	0.4570	−0.0188	0.1097	0.0655	0.0157	0.0027	0.0707	0.4325	1.2777	3.2035	11.2859	0.5066E−04
200.0	0.5915	−0.0216	0.1437	0.0718	0.0047	0.0024	0.0867	0.5762	1.8202	7.4881	12.4723	0.1125E−03
250.0	0.7288	−0.0007	−0.0276	0.1696	0.0777	0.0041	0.0003	0.1239	0.6760	2.1382	14.5119	0.8485E−04
295.0	0.8537	−0.0016	−0.0315	0.1886	0.0812	0.0048	0.0201	0.1525	0.7652	2.3017	15.4648	0.6420E−04

(*b*) S

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2665	−0.0030	0.0280	0.0145	0.0039	−0.0007	0.0348	0.3338	1.7425	20.7359	45.8217	0.8758E−04
80.0	0.2832	−0.0032	0.0296	0.0150	0.0056	−0.0025	0.0378	0.3523	1.8720	27.8824	42.9297	0.9462E−04
90.0	0.3007	−0.0035	0.0308	0.0155	0.0042	−0.0008	0.0417	0.3658	1.8893	22.1676	46.5580	0.8831E−04
100.0	0.3189	−0.0037	0.0323	0.0160	0.0049	−0.0017	0.0451	0.3841	1.9990	26.1122	46.1443	0.9152E−04
150.0	0.4173	−0.0050	0.0393	0.0183	0.0052	−0.0014	0.0623	0.4720	2.3354	25.2640	42.8032	0.8428E−04
200.0	0.5237	−0.0060	0.0464	0.0202	0.0047	−0.0005	0.0774	0.5708	2.7802	27.2320	46.4154	0.8351E−04
250.0	0.6345	−0.0070	0.0525	0.0218	0.0041	0.0008	0.0923	0.6658	3.0567	20.8530	43.1903	0.7707E−04
295.0	0.7363	−0.0078	0.0579	0.0230	0.0044	0.0008	0.1052	0.7536	3.3516	19.7461	47.9704	0.7705E−04

Table 13. *Absorptive scattering factors for ZnSe and s up to 6.0 Å^{-1}*

(*a*) Zn

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2906	−0.0132	0.0798	0.0568	0.0111	0.0004	0.0459	0.2866	1.0479	3.9572	11.4224	0.4938E−04
80.0	0.3175	−0.0154	0.0757	0.0540	0.0257	0.0020	0.0529	0.2871	0.8219	2.2372	11.3723	0.2483E−04
90.0	0.3454	−0.0158	0.0854	0.0597	0.0186	0.0013	0.0559	0.3223	0.9967	2.8832	11.8502	0.2774E−04
100.0	0.3741	−0.0157	0.1003	0.0648	0.0089	−0.0023	0.0576	0.3721	1.3561	8.1823	17.9691	0.7084E−04
150.0	0.5249	−0.0204	0.1211	0.0626	0.0232	0.0022	0.0792	0.4949	1.3155	3.0474	24.1422	0.8569E−04
200.0	0.6820	−0.0237	0.1564	0.0569	0.0246	0.0017	0.0978	0.6546	1.6685	3.3792	27.4872	0.1609E−03
250.0	0.8418	−0.0009	−0.0303	0.1922	0.0756	0.0031	0.0038	0.1412	0.7777	2.4667	25.2667	0.9912E−04
295.0	0.9869	−0.0023	−0.0348	0.2109	0.0807	0.0045	0.0317	0.1789	0.8694	2.5760	21.6476	0.6704E−04

(*b*) Se

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2029	−0.0096	0.0833	0.0534	0.0071	0.0006	0.0237	0.2300	1.0308	8.6977	32.3167	0.1597E−03
80.0	0.2204	−0.0109	0.0879	0.0564	0.0074	0.0011	0.0283	0.2430	1.0514	8.2342	23.9325	0.1650E−03
90.0	0.2386	−0.0123	0.0922	0.0596	0.0076	0.0018	0.0329	0.2558	1.0637	7.5818	19.0424	0.1704E−03
100.0	0.2574	−0.0167	0.0805	0.0594	0.0270	0.0057	0.0439	0.2312	0.6812	1.9718	15.6207	0.1207E−03
150.0	0.3568	−0.0193	0.1196	0.0745	0.0020	0.0109	0.0556	0.3482	1.2114	4.7449	8.3970	0.1614E−03
200.0	0.4610	−0.0232	0.1429	0.0752	0.0098	0.0120	0.0701	0.4390	1.3275	2.6281	10.2809	0.1896E−03
250.0	0.5675	−0.0258	0.1807	0.1532	−0.0894	0.0233	0.0823	0.5573	2.2336	2.9062	8.2689	0.2584E−03
295.0	0.6644	−0.0015	−0.0342	0.1850	0.0954	0.0173	0.0111	0.1223	0.5795	1.6663	9.7009	0.1903E−03

Table 14. *Absorptive scattering factors for ZnTe and s up to 6.0 Å^{-1}*

(*a*) Zn

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.3745	−0.0159	0.0990	0.0651	0.0092	−0.0013	0.0582	0.3687	1.3105	6.5755	17.8780	0.5998E−04
80.0	0.4129	−0.0168	0.1096	0.0669	0.0162	−0.0110	0.0629	0.4119	1.4927	13.3306	17.3517	0.8275E−04
90.0	0.4524	−0.0180	0.1173	0.0689	0.0464	−0.0409	0.0684	0.4479	1.5698	14.1022	15.1117	0.7987E−04
100.0	0.4928	−0.0193	0.1229	0.0708	0.0077	0.0001	0.0744	0.4797	1.5724	7.2244	12.7920	0.7318E−04
150.0	0.7021	−0.0017	−0.0290	0.1508	0.0873	0.0114	0.0196	0.1342	0.6078	1.7060	6.3766	0.3632E−04
200.0	0.9180	−0.0030	−0.0344	0.1915	0.0887	0.0072	0.0377	0.1778	0.7862	2.2047	11.5898	0.3791E−04
250.0	1.1367	−0.0038	−0.0402	0.2234	0.0901	0.0068	0.0493	0.2207	0.9444	2.5520	15.7575	0.5007E−04
295.0	1.3348	−0.0047	−0.0456	0.2445	0.0939	0.0081	0.0604	0.2629	1.0669	2.7059	13.7127	0.3378E−04

Table 14 (*cont.*)

(*b*) Te

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.2567	−0.0290	0.2370	0.1092	0.0178	−0.0017	0.0349	0.2815	1.3734	9.8405	69.8115	0.3682E−03
80.0	0.2853	−0.0337	0.2520	0.1171	0.0204	−0.0014	0.0415	0.3001	1.3901	8.6955	61.9313	0.3185E−03
90.0	0.3145	−0.0401	0.2536	0.1208	0.0393	0.0009	0.0494	0.3062	1.1367	4.4607	58.9585	0.1278E−03
100.0	0.3441	−0.0398	0.2878	0.1301	0.0197	−0.0045	0.0509	0.3505	1.6255	12.5843	52.3677	0.3415E−03
150.0	0.4967	−0.0521	0.3616	0.1554	0.0197	−0.0027	0.0718	0.4741	2.0136	14.1595	48.1796	0.2876E−03
200.0	0.6527	−0.0606	0.4234	0.1697	0.0234	−0.0013	0.0898	0.6003	2.2785	10.8514	37.0206	0.3502E−03
250.0	0.8103	−0.0020	−0.0733	0.4920	0.1901	0.0105	0.0000	0.1251	0.7169	2.8382	24.8469	0.3681E−03
295.0	0.9528	−0.0704	0.5525	0.2372	−0.0620	0.0106	0.1185	0.8720	3.6520	4.4247	26.5524	0.6920E−03

Table 15. *Absorptive scattering factors for CdTe and s up to 6.0 Å^{-1}*

(*a*) Cd

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.4900	−0.0457	0.2975	0.1157	0.0150	0.0299	0.0718	0.4554	1.6230	1.6532	6.3555	0.1721E−03
80.0	0.5504	−0.0488	0.3150	0.1186	0.0441	0.0098	0.0790	0.5019	1.5518	3.7480	11.6566	0.2151E−03
90.0	0.6116	−0.0507	0.3485	0.1367	0.0223	0.0061	0.0850	0.5639	1.9918	6.5298	10.5764	0.2715E−03
100.0	0.6734	−0.0531	0.3725	0.1407	0.0275	−0.0024	0.0915	0.6179	2.1861	8.0573	13.6782	0.3225E−03
150.0	0.9876	−0.0101	−0.0798	0.4414	0.1915	0.0414	0.0471	0.1938	0.7739	2.2466	7.6946	0.1481E−03
200.0	1.3060	−0.0108	−0.0902	0.5382	0.2018	0.0236	0.0562	0.2420	1.0186	3.0972	12.0682	0.1179E−03
250.0	1.6262	−0.0136	−0.1100	0.5565	0.2476	0.0481	0.0712	0.3153	1.1615	2.8609	9.8556	0.3237E−03
295.0	1.9151	−0.0124	−0.1091	0.6653	0.2168	0.0171	0.0735	0.3383	1.4340	4.1030	19.8815	0.1497E−03

(*b*) Te

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.3360	−0.0409	0.2736	0.1286	0.1023	−0.0752	0.0515	0.3321	1.3652	8.4851	9.5652	0.2017E−03
80.0	0.3757	−0.0470	0.2730	0.0924	0.0613	0.0336	0.0594	0.3461	0.9747	1.8332	5.2699	0.1071E−03
90.0	0.4160	−0.0487	0.3083	0.1384	0.0367	0.0028	0.0637	0.3912	1.4331	5.0487	14.7406	0.1216E−03
100.0	0.4569	−0.0520	0.3163	0.0954	0.0814	0.0196	0.0692	0.4178	1.1556	2.3797	8.7647	0.1463E−03
150.0	0.6656	−0.0022	−0.0708	0.4142	0.1854	0.0332	0.0007	0.1126	0.5717	1.9963	7.9998	0.1037E−03
200.0	0.8778	−0.0693	0.5102	0.1782	0.0096	0.0129	0.1127	0.7913	2.8244	8.2104	13.6623	0.5961E−03
250.0	1.0916	−0.0083	−0.0893	0.5710	0.2199	0.0185	0.0400	0.1884	0.8979	3.0658	18.6827	0.1935E−03
295.0	1.2847	−0.0098	−0.0967	0.6314	0.2250	0.0149	0.0484	0.2203	1.0426	3.4882	22.0378	0.2430E−03

Table 16. *Absorptive scattering factors for HgSe and s up to 6.0 Å^{-1}*

(*a*) Hg

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.9272	−0.0065	−0.1650	1.1447	0.2923	0.0120	0.0091	0.1413	0.7795	2.8838	44.0494	0.5778E−03
80.0	1.0538	−0.0121	−0.1767	1.2251	0.2995	0.0132	0.0275	0.1669	0.8623	3.1103	45.4376	0.5108E−03
90.0	1.1809	−0.0171	−0.1883	1.2934	0.3101	0.0138	0.0392	0.1929	0.9409	3.2567	38.6910	0.4365E−03
100.0	1.3084	−0.0187	−0.1967	1.3686	0.3049	0.0087	0.0440	0.2119	1.0298	3.5759	37.7547	0.4486E−03
150.0	1.9493	−0.0264	−0.2347	1.6417	0.3091	0.0103	0.0666	0.3113	1.4338	4.5746	35.5627	0.2751E−03
200.0	2.5927	−0.0302	−0.2575	1.8411	0.3029	0.0118	0.0835	0.3992	1.8268	5.4323	26.6671	0.2275E−03
250.0	3.2371	−0.0309	−0.2646	0.0032	2.0364	0.2541	0.0950	0.4679	1.3954	2.2525	7.3047	0.3627E−03
295.0	3.8175	−0.0162	−0.0458	−0.2609	2.1603	0.2573	0.0799	0.2310	0.6057	2.5682	7.9829	0.2802E−03

(*b*) Se

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.4008	−0.0217	0.1225	0.0746	0.0187	0.0066	0.0631	0.3736	1.0916	3.0908	16.0780	0.1238E−03
80.0	0.4458	−0.0222	0.1460	0.0769	0.0086	0.0037	0.0672	0.4380	1.4923	8.4896	24.4115	0.1553E−03
90.0	0.4916	−0.0234	0.1614	0.0762	0.0083	0.0024	0.0724	0.4883	1.7080	13.1902	39.6379	0.1759E−03
100.0	0.5381	−0.0246	0.1754	0.0752	0.0078	0.0023	0.0779	0.5364	1.8924	16.7592	35.2144	0.2004E−03
150.0	0.7766	−0.0309	0.2351	0.0698	0.0086	0.0006	0.1061	0.7598	2.6795	20.9260	35.7173	0.2649E−03
200.0	1.0204	−0.0366	0.2844	0.0655	0.0031	0.0069	0.1343	0.9651	3.4871	16.3375	36.2383	0.3697E−03
250.0	1.2665	−0.0416	0.3266	0.0632	−0.0040	0.0115	0.1623	1.1594	4.4542	14.3425	27.9757	0.4460E−03
295.0	1.4891	−0.0445	0.3651	0.6838	−0.6335	0.0113	0.1832	1.3474	8.3530	8.6526	43.1330	0.5035E−03

Table 17. *Absorptive scattering factors for HgTe and s up to 6.0 Å^{-1}*

(*a*) Hg

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	1.3316	−0.0284	−0.2168	1.2963	0.3730	0.0526	0.0576	0.2439	0.9825	2.6564	9.1126	0.9421E−04
80.0	1.5159	−0.0306	−0.2341	1.3361	0.4053	0.0772	0.0641	0.2770	1.0786	2.5954	8.5996	0.3419E−03
90.0	1.7008	−0.0330	−0.2554	1.2982	0.5009	0.1108	0.0705	0.3136	1.1455	2.3639	7.7979	0.4983E−03
100.0	1.8861	−0.0321	−0.2586	1.3640	0.4830	0.1243	0.0731	0.3334	1.2686	2.4920	7.4763	0.3440E−03
150.0	2.8159	−0.0321	−0.2697	1.7384	0.3143	0.1652	0.0901	0.4360	1.8985	3.3391	7.8779	0.3003E−03
200.0	3.7482	−0.0353	−0.2800	2.1030	0.2845	0.0127	0.1111	0.5474	2.5109	6.8900	26.9696	0.2872E−03
250.0	4.6815	−0.0395	−0.2907	2.2397	0.2824	0.0207	0.1348	0.6672	3.0323	7.5000	22.7378	0.3119E−03
295.0	5.5220	−0.0433	−0.2965	2.3398	0.2816	0.0236	0.1566	0.7755	3.4933	8.1002	23.4576	0.3198E−03

(*b*) Te

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.4448	−0.0506	0.3233	0.1439	0.0361	0.0013	0.0671	0.4162	1.5352	5.6901	49.6716	0.1379E−03
80.0	0.5002	−0.0542	0.3466	0.1476	0.0412	0.0029	0.0739	0.4607	1.6128	5.2906	49.4400	0.1773E−03
90.0	0.5563	−0.0573	0.3686	0.1497	0.0474	0.0038	0.0803	0.5059	1.6806	5.0341	52.3741	0.2454E−03
100.0	0.6127	−0.0597	0.3960	0.1563	0.0421	0.0033	0.0863	0.5566	1.8855	5.6463	52.2781	0.3079E−03
150.0	0.8994	−0.0703	0.5101	0.1538	0.0523	0.0035	0.1151	0.8040	2.5039	5.7611	52.5218	0.6407E−03
200.0	1.1897	−0.0789	0.6202	0.1782	0.0169	0.0033	0.1432	1.0567	3.6386	12.3273	37.3180	0.8686E−03
250.0	1.4814	−0.0866	0.7161	0.1723	0.0065	0.0066	0.1710	1.3024	4.6366	12.9508	43.0911	0.1058E−02
295.0	1.7447	−0.0116	−0.1113	0.7647	0.2209	0.0109	0.0624	0.2897	1.3890	4.5959	49.8153	0.2895E−03

Table 18. *Absorptive scattering factors for CuCl and s up to 6.0 Å^{-1}*

(*a*) Cu

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.9239	−0.0019	−0.0316	0.1910	0.0785	0.0028	0.0275	0.1667	0.8246	2.4587	13.3283	0.1174E−03
80.0	1.0386	−0.0035	−0.0361	0.1972	0.0878	0.0071	0.0466	0.2048	0.8715	2.3239	8.5200	0.7684E−04
90.0	1.1548	−0.0050	−0.0431	0.1828	0.1104	0.0197	0.0597	0.2490	0.8696	1.9232	5.5542	0.6752E−04
100.0	1.2721	−0.0054	−0.0478	0.1630	0.1333	0.0330	0.0651	0.2766	0.8862	1.7026	4.6133	0.1010E−03
150.0	1.8679	−0.0054	−0.0556	0.2392	0.1237	0.0224	0.0785	0.3607	1.3301	2.4577	7.3854	0.4937E−04
200.0	2.4712	−0.0056	−0.0606	0.3244	0.0890	0.0131	0.0929	0.4401	1.7832	3.6019	11.8461	0.4483E−04
250.0	3.0776	−0.0059	−0.0641	0.3734	0.0726	0.0123	0.1065	0.5143	2.1789	4.4561	13.8901	0.5338E−04
295.0	3.6248	−0.0065	−0.0665	0.4034	0.0656	0.0129	0.1221	0.5833	2.5059	5.0279	14.8487	0.5692E−04

(*b*) Cl

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.6546	−0.0081	0.0530	0.0250	0.0105	0.0015	0.0942	0.6283	2.0079	6.4336	24.1264	0.4962E−04
80.0	0.7236	−0.0084	0.0594	0.0275	0.0086	−0.0008	0.1012	0.7085	2.5817	10.9667	20.2190	0.6048E−04
90.0	0.7939	−0.0088	0.0641	0.0285	0.0091	−0.0020	0.1089	0.7775	2.8827	13.1571	21.6234	0.7174E−04
100.0	0.8654	−0.0093	0.0687	0.0296	0.0098	−0.0036	0.1174	0.8460	3.2135	16.1598	23.6986	0.8292E−04
150.0	1.2339	−0.0014	−0.0142	0.0813	0.0376	0.0114	0.0532	0.2358	1.0380	3.1987	11.1154	0.2057E−04
200.0	1.6126	−0.0019	−0.0180	0.0906	0.0440	0.0164	0.0716	0.3202	1.2546	3.2837	10.7264	0.2249E−04
250.0	1.9963	−0.0018	−0.0187	0.1137	0.0427	0.0089	0.0759	0.3588	1.6288	5.0762	14.8613	0.2402E−04
295.0	2.3439	−0.0020	−0.0211	0.1216	0.0449	0.0125	0.0887	0.4257	1.8377	5.1334	13.8512	0.1471E−04

Table 19. *Absorptive scattering factors for CuBr and s up to 6.0 Å^{-1}*

(*a*) Cu

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.5397	−0.0194	0.1256	0.0698	0.0085	−0.0029	0.0802	0.5260	1.6918	8.9753	25.4675	0.1047E−03
80.0	0.6008	−0.0209	0.1352	0.0695	0.0098	−0.0012	0.0882	0.5801	1.7355	6.1055	22.6996	0.1285E−03
90.0	0.6630	−0.0220	0.1518	0.0693	0.0105	−0.0076	0.0952	0.6508	2.0714	18.2691	30.7250	0.1483E−03
100.0	0.7262	−0.0233	0.1626	0.0688	0.0198	−0.0164	0.1028	0.7083	2.1728	16.9816	22.2761	0.1816E−03
150.0	1.0503	−0.0292	0.2211	0.0579	0.0064	−0.0026	0.1407	1.0090	3.0297	12.2709	22.0343	0.2889E−03
200.0	1.3814	−0.0347	0.2692	0.0479	0.0059	−0.0020	0.1796	1.2811	3.9172	11.0630	22.3682	0.3731E−03
250.0	1.7155	−0.0394	0.3088	0.0428	−0.0001	0.0018	0.2166	1.5349	5.0738	19.2189	25.1980	0.4221E−03
295.0	2.0175	−0.0048	−0.0531	0.3163	0.0715	0.0046	0.0767	0.3607	1.5706	4.0448	20.0833	0.3345E−04

Table 19 (*cont.*)

(*b*) Br

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.7337	−0.0031	−0.0393	0.2066	0.1043	0.0212	0.0273	0.1431	0.6198	1.6815	7.9433	0.5549E−04
80.0	0.8247	−0.0033	−0.0416	0.2325	0.1003	0.0190	0.0305	0.1568	0.7027	1.9590	9.5956	0.5473E−04
90.0	0.9168	−0.0022	−0.0422	0.2680	0.0871	0.0125	0.0211	0.1583	0.8141	2.5966	15.2837	0.1064E−03
100.0	1.0099	−0.0019	−0.0436	0.2944	0.0807	0.0090	0.0190	0.1667	0.9068	3.1934	23.5105	0.1523E−03
150.0	1.4825	−0.0046	−0.0559	0.3687	0.0831	0.0092	0.0531	0.2542	1.2265	4.2391	24.1141	0.1125E−03
200.0	1.9612	−0.0055	−0.0629	0.4313	0.0799	0.0045	0.0678	0.3200	1.5605	5.8666	28.0859	0.1242E−03
250.0	2.4423	−0.0066	−0.0699	0.4715	0.0836	0.0082	0.0840	0.3937	1.8468	6.3461	22.4451	0.7005E−04
295.0	2.8765	−0.0079	−0.0762	0.4897	0.0892	0.0214	0.0999	0.4664	2.0653	5.6785	15.4266	0.6145E−04

Table 20. *Absorptive scattering factors for CuI and s up to 6.0 Å^{-1}*

(*a*) Cu

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.6486	−0.0007	−0.0252	0.1397	0.0787	0.0078	0.0002	0.1150	0.5863	1.7568	6.2072	0.1044E−03
80.0	0.7245	−0.0031	−0.0300	0.1351	0.0890	0.0207	0.0355	0.1550	0.5874	1.4834	3.9983	0.1240E−03
90.0	0.8017	−0.0045	−0.0338	0.1377	0.0984	0.0249	0.0473	0.1835	0.6161	1.4605	3.9520	0.1150E−03
100.0	0.8800	−0.0050	−0.0371	0.1439	0.1056	0.0257	0.0523	0.2039	0.6588	1.5116	4.1550	0.9905E−04
150.0	1.2803	−0.0054	−0.0483	0.1656	0.1331	0.0319	0.0657	0.2794	0.8913	1.7292	4.6844	0.1037E−03
200.0	1.6879	−0.0052	−0.0522	0.2438	0.1089	0.0165	0.0736	0.3309	1.2485	2.5606	8.1590	0.3925E−04
250.0	2.0987	−0.0053	−0.0559	0.3098	0.0830	0.0079	0.0828	0.3836	1.5802	3.6443	14.6653	0.2930E−04
295.0	2.4697	−0.0056	−0.0609	0.2969	0.1084	0.0213	0.0925	0.4398	1.7413	3.0566	9.2431	0.5891E−04

(*b*) I

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.3602	−0.0409	0.2928	0.1425	0.0321	−0.0089	0.0523	0.3602	1.4687	9.3697	40.4931	0.3430E−03
80.0	0.4031	−0.0451	0.3139	0.1488	0.0354	−0.0081	0.0589	0.3944	1.5310	8.5478	36.2428	0.2924E−03
90.0	0.4467	−0.0477	0.3444	0.1535	0.0365	−0.0157	0.0641	0.4394	1.7910	12.6546	30.2993	0.3425E−03
100.0	0.4908	−0.0498	0.3755	0.1562	0.0558	−0.0420	0.0688	0.4869	2.1053	22.4770	32.4270	0.4156E−03
150.0	0.7159	−0.0636	0.4788	0.1732	0.0444	−0.0323	0.0961	0.6775	2.7082	20.6644	36.2987	0.5177E−03
200.0	0.9448	−0.0746	0.5672	0.1835	0.0410	−0.0291	0.1216	0.8649	3.2689	20.1379	37.2672	0.7438E−03
250.0	1.1753	−0.0833	0.6441	0.1882	0.0536	−0.0411	0.1455	1.0492	3.7682	19.9085	32.1579	0.9445E−03
295.0	1.3834	−0.0902	0.7089	0.1904	0.0640	−0.0554	0.1669	1.2151	4.2680	24.2422	36.6946	0.1079E−02

Table 21. *Absorptive scattering factors for SiC and s up to 6.0 Å^{-1}*

(*a*) Si

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.1328	−0.0014	0.0096	0.0076	0.0039	0.0015	0.0176	0.1500	0.5191	1.7024	10.6425	0.1244E−04
80.0	0.1343	−0.0014	0.0098	0.0078	0.0037	0.0014	0.0168	0.1544	0.5479	1.8494	11.4842	0.1228E−04
90.0	0.1361	−0.0014	0.0098	0.0079	0.0038	0.0014	0.0181	0.1539	0.5409	1.8492	11.9076	0.1252E−04
100.0	0.1382	−0.0015	0.0100	0.0080	0.0038	0.0014	0.0187	0.1557	0.5474	1.8784	12.2759	0.1297E−04
150.0	0.1528	−0.0017	0.0108	0.0088	0.0040	0.0015	0.0228	0.1673	0.5787	2.0328	14.0428	0.1513E−04
200.0	0.1725	−0.0014	0.0141	0.0098	0.0020	0.0008	0.0174	0.2204	0.9715	6.7657	11.8384	0.3054E−04
250.0	0.1954	−0.0021	0.0143	0.0108	0.0032	0.0013	0.0293	0.2197	0.8180	3.5568	17.3672	0.1456E−04
295.0	0.2179	−0.0027	0.0141	0.0117	0.0047	0.0017	0.0378	0.2200	0.7067	2.5834	16.3257	0.1216E−04

(*b*) C

T (K)	B	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	σ
70.0	0.1714	−0.0003	0.0027	0.0019	0.0013	0.0001	0.0221	0.2079	0.9371	4.3847	24.0456	0.3663E−05
80.0	0.1726	−0.0003	0.0027	0.0019	0.0013	0.0002	0.0229	0.2075	0.9219	4.2244	21.7815	0.3523E−05
90.0	0.1740	−0.0003	0.0031	0.0021	0.0016	−0.0008	0.0133	0.2392	1.4664	11.9909	17.3401	0.9328E−05
100.0	0.1755	−0.0003	0.0031	0.0022	0.0018	−0.0011	0.0122	0.2450	1.5675	14.5771	20.4464	0.1088E−04
150.0	0.1850	−0.0003	0.0032	0.0023	0.0015	−0.0008	0.0162	0.2515	1.5709	13.5847	21.0216	0.1069E−04
200.0	0.1971	−0.0003	0.0033	0.0024	0.0015	−0.0006	0.0212	0.2567	1.5025	11.0272	17.8834	0.9120E−05
250.0	0.2115	−0.0003	0.0036	0.0026	0.0013	−0.0006	0.0223	0.2795	1.7529	15.3983	27.9356	0.1262E−04
295.0	0.2261	−0.0005	0.0035	0.0025	0.0013	0.0000	0.0324	0.2673	1.3306	6.7083	20.2835	0.5603E−05

Since our data file for elastic scattering factors does not contain data for $s > 6.0\,\text{Å}^{-1}$ and for ions for all values of s, we have developed another two general-purpose programs for the parameterization of all other scattering factors. To use these programs, a data file containing m numerical scattering factors and corresponding s values should be prepared first by the user. The first general-purpose program *ELASGEN* then reads this data file and uses the routine *MCFIT* to fit these data with five Gaussians (the data file can also be a file for X-ray scattering factors). If the scattering factors are for electrons, the second general-purpose program *ABSORGEN* then calculates the corresponding absorptive scattering factors using the routine of Dudarev *et al.* (1995) and returns a_j and b_j.

4. Conclusions

In this paper, a robust algorithm and computer programs have been developed for parameterization of numerical atomic scattering factors. The programs have been applied successfully to fit both the elastic and the absorptive structure factors for all neutral atoms for s up to $6.0\,\text{Å}^{-1}$ and all Debye–Waller factors with high accuracy. For elastic scattering factors, two tables have been given of the electron scattering factors for all neutral atoms and for two ranges of $s = 0 \rightarrow 2\,\text{Å}^{-1}$ and $s = 0 \rightarrow 6\,\text{Å}^{-1}$. Error analysis has been made and compared with previous results obtained by others. In terms of the roots of the mean squares, it is shown that for all neutral atoms the results presented in the present paper are considerably more accurate than the previous analytical fittings. Results for the parameterization of absorptive scattering factors for 17 important materials with the zinc blende structure have been tabulated over the temperature range of 1 to 1000 K. These materials are GaP, GaSb, GaAs, InP, InSb, InAs, ZnO, ZnS, ZnSe, ZnTe, CdTe, HgSe, HgTe, CuCl, CuBr, CuI and SiC. For other materials and temperatures, the parameterization can be caried out using our program by providing the atomic number of the element, the Debye–Waller factor and the acceleration voltage and the program will be made freely available *via* electronic mail from lmpeng@lmplab.blem.ac.cn or on floppy disk upon request.

As a by-product of the present study, two misprints have been identified in Table 4(*a*) of Doyle & Turner (1968). These misprints occur for Eu and Rn with atomic numbers 63 and 86, respectively.

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