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**A useful analytic approximation to atomic and unitary atomic scattering factors.** By J. N. SILVERMAN and S. H. SIMONSEN, *Department of Chemistry, The University of Texas, Austin, Texas, U.S.A.*

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### Introduction

For the past two years we have been using an analytic approximation to the atomic scattering factor suggested by Steinfink (1957),\*

$$f_0(x) = \exp(\sum \alpha_n x^n), \quad (1)$$

where  $f_0$  is the temperature-uncorrected atomic scattering factor and  $x = \sin \theta/\lambda$ . This may be written as

$$\log_e f_0(x) = \sum_n \alpha_n x^n, \quad (2)$$

i.e., a polynomial of the  $n$ th degree in  $x$ . This function has been found to have the following important advantages:

(a) The evaluation of the best parameters is simple and straightforward because of their linear form in equation (2).

(b) Unlike some other analytic approximations (Vand, Eiland & Pepinsky, 1957; Freeman & Smith, 1958), function (1) is not restricted to the Cu  $K\alpha$  scattering range but reproduces the scattering curves tested with good accuracy over the entire Mo  $K\alpha$  range.

(c) The effect of thermal motion on  $f_0$  can be simply introduced by subtraction of the appropriate temperature factor  $B$  from  $\alpha_2$ , the coefficient of  $x^2$ .

(d) It will be shown that the unitary atomic scattering factors  $\hat{f}_0$  and  $\hat{f}$ , and the quantity  $\sum_j \hat{f}_0^2_j$  can be conveniently approximated with an expression of the form of equation (1).

Function (1) was tested on eleven atoms and ions. Two essentially different types of parameters, designated as least-squares parameters and unique polynomial coefficients, were determined in each case.

### Least-squares parameters

To cover the entire scattering range, a sixth-degree polynomial was used as an exponent in (1).  $\alpha_0$  was determined by the condition that  $\exp \alpha_0 = f_0(0) = N$  where  $N$  is the number of electrons in the atom or ion. The remaining parameters were determined by the usual least-squares technique minimizing the expression

$$\sum_t (\log_e f_t - \log_e f_0)^2$$

where the  $f_0$ 's are the calculated values and the  $f_t$ 's are the tabulated values fitted. A standard deviation,  $\sigma$ , given by

$$\sigma = \left[ \sum_{t=1}^m (\Delta f_0)_t^2 / m \right]^{1/2},$$

\* To our knowledge, Dr Hugo Steinfink of the Shell Development Company, Houston, Texas, first used equation (1) to obtain a least-squares fit of certain atomic scattering factors. His degree of fit is somewhat less than ours as he employed a smaller number of parameters.

was used as a criterion of fit. The normal equations were solved by Crout's (1941) procedure, including an iterative process to reduce the effect of round-off error. One set of parameters was derived for a scattering range sufficient to include Cu  $K\alpha$  radiation and a different set to include the larger Mo  $K\alpha$  range. These parameters are collected in Table 1 with  $\sigma$ ,  $\sigma/N$  and the mean relative error

$$\bar{r} = \sum_{t=1}^m |\Delta f_0 / f_0|_t / m.$$

Occasionally, the Mo  $K\alpha$  parameters fitted the Cu  $K\alpha$  range as well as the parameters directly derived for the smaller range. In such cases, only the former values are listed.

### Coefficients of unique polynomials

Each scattering curve was divided into successive angular ranges containing six tabulated points. Each such range was then precisely fitted by a unique fifth-degree polynomial in equation (1) containing, in general, six independent constants. An overlap of adjacent ranges, usually by one point, was taken to ensure continuity in the values. The amount of overlap was sometimes varied to obtain the best possible fit. These coefficients and their range of applicability are presented in Table 2.

### Accuracy of representation

The data in Table 1 shows that a sixth-degree polynomial is sufficient to give a good least-squares fit of  $f_0$  over a wide range of  $\sin \theta/\lambda$ . The somewhat larger deviations observed for C in the Mo  $K\alpha$  range and Cl<sup>-</sup> in both ranges indicate that occasionally a polynomial exponent of higher degree is required to obtain an equivalent degree of accuracy throughout. Raising the degree of the exponent, however, would not greatly increase the computations necessary. The heavier atoms and ions fitted, which scatter significantly to large values of  $\sin \theta/\lambda$ , are particularly well represented throughout the entire Mo  $K\alpha$  range. This is illustrated in Table 3 for the typical case of Zn. Here we have compared our calculated values of  $f_0$  for the Mo  $K\alpha$  range with the tabulated values and with the values calculated with the analytic approximation of Forsyth & Wells (1959). The relative errors are also listed.

The unique fifth-degree polynomial coefficients in Table 2 reproduce the tabulated  $f_0$  values in the appropriate interval without error. An estimation of the error due to polynomial interpolation (Milne, 1949, pp. 78 ff. and p. 128) with a fifth-degree polynomial in equation (2) showed that in general it was insufficient to influence the last significant figure of  $f_0$ . Therefore, the interpolated values derived from these coefficients are as accurate as the tabulated ones from which they are obtained.

Table 1. *Least-squares parameters*

	$N$	Range of $\sin \theta/\lambda$	$\alpha_0$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\sigma$	$\sigma/N$ (%)	$\bar{r}$ (%)	Ref.
C	6	0.00-0.70	1.7918	0.42345	-25.640	64.045	-48.699	-10.709	20.000	0.010	0.17	0.15	B
		0.00-1.30	1.7918	2.1036	-44.731	140.72	-193.98	124.52	-30.380	0.095	1.58	2.64	
N	7	0.00-0.70	1.9459	-0.63334	-1.1860	-72.258	282.33	-391.74	190.00	0.025	0.36	0.43	B
		0.00-1.30	1.9459	-0.10500	-15.809	32.754	-25.197	6.4815	0.17818	0.044	0.63	1.08	
O	8	0.00-0.70	2.0794	-0.31824	-4.5467	-35.249	149.27	-203.78	97.000	0.014	0.18	0.22	B
		0.00-1.30	2.0794	0.17384	-14.047	24.327	-14.221	0.88429	1.1312	0.014	0.18	0.45	
Cl	17	0.0-0.716	2.8332	0.34045	-28.576	117.98	-217.50	192.16	-66.745	0.012	0.07	0.09	VØ
		0.0-1.353	2.8332	0.37951	-23.484	77.171	-107.64	68.306	-16.233	0.161	0.95	2.09	
Cl <sup>-</sup>	18	0.00-0.70	2.8904	2.5866	-66.900	356.48	-898.62	1088.8	-507.00	0.250	1.39	1.48	B
		0.00-1.30	2.8904	1.1373	-31.639	105.98	-153.46	101.81	-25.380	0.212	1.18	2.20	
Ni <sup>++</sup>	26	0.00-0.70	3.2581	0.24338	-9.4961	21.651	-23.960	13.144	-2.8465	0.049	0.19	0.23	TU
		0.00-1.30								0.037	0.14	0.18	
Ni	28	0.0-0.716	3.3322	-1.8574	9.0964	-57.608	143.63	-160.41	67.564	0.029	0.10	0.10	VØ
		0.0-1.353	3.3322	-1.1959	-1.3929	-0.93967	6.0001	-5.3616	1.4769	0.086	0.31	0.37	
Zn <sup>++</sup>	28	0.00-0.70	3.3322	0.22225	-9.2690	21.171	-23.483	12.917	-2.8056	0.050	0.18	0.20	TU
		0.00-1.30								0.038	0.14	0.18	
Zn	30	0.00-0.70	3.4012	-0.32689	-6.0929	12.447	-13.731	8.4050	-2.1172	0.089	0.30	0.35	B
		0.00-1.30								0.074	0.25	0.35	
Pd <sup>++</sup>	44	0.00-0.70	3.7842	0.13402	-7.5232	13.113	-2.0166	-15.083	-10.816	0.033	0.08	0.06	TU
		0.00-1.30	3.7842	0.15002	-8.2046	19.069	-21.602	12.120	-2.6790	0.045	0.10	0.15	
Pd	46	0.00-0.70	3.8286	-0.26515	-6.8628	17.113	-20.284	11.788	-2.6800	0.137	0.30	0.29	TU
		0.00-1.30								0.104	0.23	0.24	

B: Berghuis *et al.* (1955). TU: Thomas & Umeda (1957). VØ: Viervoll & Øgrim (1949).

Table 2. *Coefficients of unique fifth-degree polynomials*

	<i>N</i>	Range of $\sin \theta/\lambda$	$\alpha_0$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$
C	6	0.00 -0.25	1.79176	0.101999	-19.7406	33.4898	-12.0397	40.8497
		0.25 -0.60	2.43441	-6.97155	6.28525	1.36236	-0.596875	-3.78245
		0.50 -1.00	1.81768	-4.51004	4.25111	0.984194	-4.38583	1.93450
		0.80 -1.30	0.422278	0.926590	-1.98854	0.693644	0.172529	-0.135592
N	7	0.00 -0.25	1.94591	-0.0339148	-11.8993	-7.68009	106.042	-141.637
		0.25 -0.60	2.11402	-2.00200	-5.44384	-0.991157	30.4335	-27.6963
		0.50 -1.00	3.37380	-11.1501	15.6765	-8.55028	-0.381498	1.26506
		0.80 -1.30	4.32485	-13.1371	15.2879	-5.62264	-1.83560	1.21663
O	8	0.00 -0.25	2.07944	-0.0326747	-9.54497	-6.12299	73.8164	-98.1579
		0.25 -0.60	1.77179	4.46131	-36.5769	80.5341	-82.1795	33.9371
		0.60 -1.10	1.87171	0.522783	-13.9071	25.5511	-18.6376	4.91698
		0.80 -1.30	1.82436	-3.17296	2.31004	-0.432614	-0.308553	0.0976961
Cl	17	0.000-0.398	2.83321	0.549344	-33.2288	150.824	-303.166	239.135
		0.398-0.796	2.93948	-3.09420	-0.0397026	12.7681	-21.0753	10.0290
		0.637-1.035	1.96230	0.755137	-0.848583	-2.41316	-2.65479	-0.749357
		0.955-1.353	2.45578	-1.56126	1.44170	-0.928000	-0.376154	0.330000
Cl <sup>-</sup>	18	0.00 -0.25	2.89037	0.0710735	-18.6737	41.1345	12.8878	-77.9083
		0.25 -0.60	3.90706	-13.3958	48.0850	-103.586	120.222	-57.8612
		0.60 -1.10	2.01219	1.79054	-6.68367	8.55823	-5.94969	1.66116
		0.80 -1.30	0.508276	6.14430	-8.41507	2.77732	0.902006	-0.528622
Ni <sup>++</sup>	26	0.00 -0.25	3.25810	-0.0114928	-4.79774	-7.30335	54.6459	-73.2742
		0.15 -0.40	3.18731	1.39426	-15.7536	36.0479	-37.3237	14.8284
		0.40 -0.65	3.51889	-1.60293	-5.57054	20.0190	-25.8102	11.8103
		0.65 -0.90	8.60059	-25.7104	36.2103	-12.4196	-13.6603	9.01214
		0.90 -1.15	2.81265	-0.142995	-1.17437	0.500927	-0.00319618	0.00167374
		1.05 -1.30	2.97851	-0.959403	-0.0419709	-0.0503121	0.0817473	-0.0158425
Ni	28	0.000-0.398	3.33220	-2.02062	12.1975	-75.1835	173.529	-140.092
		0.080-0.477	3.30679	-1.29136	4.67279	-39.4646	94.3251	-73.7433
		0.477-0.875	3.29540	-1.24967	-1.59415	2.27665	-1.16501	0.386152
		0.637-1.035	3.34328	-1.75275	0.810396	-3.25668	4.75395	-1.97800
		0.955-1.353	3.56349	-2.46473	0.842948	-0.246000	0.401538	-0.180000
Zn <sup>++</sup>	28	0.00 -0.25	3.33220	-0.0206554	-4.60561	-8.98146	63.0479	-87.0613
		0.15 -0.40	3.35941	-0.638290	0.462568	-26.1220	78.7263	-69.5593
		0.40 -0.65	3.61756	-2.16161	-2.30388	12.4931	-17.9821	8.80769
		0.65 -0.90	5.85560	-12.5933	16.0408	-4.32147	-7.29550	4.41724
		0.90 -1.15	2.72399	-0.0387937	-0.0709542	-1.78563	1.70471	-0.452657
		1.05 -1.30	2.78551	0.0552122	-1.35414	0.641632	-0.00172315	-0.0423486
Zn	30	0.00 -0.25	3.40120	0.0652945	-12.9794	48.3093	-75.2946	18.9993
		0.25 -0.60	3.12976	2.90664	-21.8083	51.4738	-61.8348	30.1463
		0.60 -1.10	3.62067	-1.74586	-1.08681	1.35317	0.173972	-0.324481
		0.80 -1.30	4.00097	-3.10113	0.223664	1.76793	-1.06385	0.163008
Pd <sup>++</sup>	44	0.00 -0.25	3.78419	-0.00644965	-4.76157	-5.07402	48.2748	-63.5344
		0.05 -0.30	3.78249	0.0710579	-6.03485	-4.54928	14.2997	-18.2214
		0.30 -0.55	3.64577	2.32352	-20.9927	53.7339	-64.3927	29.7685
		0.50 -0.75	4.08478	-2.17895	-1.07425	7.98901	-11.3799	5.36558
		0.75 -1.00	4.23886	-3.58108	5.30146	-6.66943	4.71156	-1.36086
		1.00 -1.25	8.24827	-15.6709	16.2633	-6.40000	-0.400000	0.600000
		1.05 -1.30	3.34820	-0.167578	-0.820505	0.122628	0.245570	-0.0884747
Pd	46	0.00 -0.25	3.82864	0.0130814	-8.90087	5.22805	92.9772	-196.981
		0.05 -0.30	3.82028	0.394756	-15.1631	52.4921	-73.6597	24.9806
		0.30 -0.55	3.75149	0.164662	-6.74574	11.8152	-7.08880	0.00534866
		0.50 -0.75	3.63859	0.208409	-4.31697	5.24461	-2.24948	0.0919988
		0.75 -1.30						

Use same coefficients given for Pd<sup>++</sup> above to cover these ranges

### Suggested applications

#### *Initial stages of structure determination*

In addition to the analytic approximation of the atomic scattering factor, equation (1) is well suited to the ready

calculation of another quantity, the unitary atomic scattering factor, which has widespread application.

Patterson (1935) suggested that the unitary atomic scattering factor,  $\hat{f}_0$ , for a given structure be calculated from the expression

Table 3. *Tabulated and calculated values of  $f_0$  for zinc ( $0 \leq \sin \theta/\lambda \leq 1.30$ )*

$\sin \theta/\lambda$	$f_0$ (tab.)	Forsyth & Wells (1959)		Least-squares fit with equation (1)	
		$f_0$ (calc.)	$  \Delta f_0 / f_0   \%$	$f_0$ (calc.)	$  \Delta f_0 / f_0   \%$
0.00	30.00	29.78	0.73	30.00	0.00
0.05	29.30	29.26	0.14	29.11	0.65
0.10	27.63	27.84	0.76	27.63	0.00
0.15	25.67	25.87	0.78	25.81	0.55
0.20	23.74	23.75	0.04	23.86	0.51
0.25	21.88	21.74	0.64	21.92	0.18
0.30	20.11	19.94	0.85	20.06	0.25
0.35	18.41	18.34	0.38	18.33	0.43
0.40	16.83	16.89	0.36	16.74	0.53
0.45	15.38*	15.54	1.04	15.32	0.39
0.50	14.05	14.26	1.49	14.04	0.07
0.55	12.86*	13.08	1.71	12.90	0.31
0.60	11.84	11.98	1.18	11.89	0.42
0.65	10.93*	11.00	0.64	10.99	0.55
0.70	10.15	10.13	0.20	10.21	0.59
0.75	9.48*	9.37	1.16	9.52	0.42
0.80	8.90	8.73	1.91	8.92	0.22
0.85	8.41*	8.20	2.50	8.40	0.12
0.90	7.99	7.77	2.75	7.96	0.38
0.95	7.63*	7.42	2.75	7.59	0.52
1.00	7.32	7.15	2.32	7.28	0.55
1.10	6.81	6.78	0.44	6.81	0.00
1.20	6.40	6.57	2.66	6.44	0.63
1.30	6.04	6.46	6.95	6.02	0.33
		$\sigma$	0.18		0.07
		$\sigma/N$ (%)	0.59		0.23
		$\bar{r}$ (%)	1.43		0.36

\* These tabulated  $f_0$  entries are interpolated values calculated with the unique polynomial coefficients of Table 2.

$$\hat{f}_0 \approx \frac{\sum_{j=1}^P f_{0j}}{\sum_{j=1}^P N_j}, \quad (3)$$

the summation, as usual, being over the contents of the unit cell. As this is only an approximation, an equally valid representation is given by the geometric mean

$$\hat{f}_0 \approx \left( \prod_{j=1}^P f_{0j} \right)^{1/P} / \left( \prod_{j=1}^P N_j \right)^{1/P} = \left[ \prod_{j=1}^P (f_{0j}/N_j) \right]^{1/P}. \quad (4)$$

Equation (4) differs but slightly from (3) for structures containing atoms of about the same atomic number, and it is just in such cases that the approximate concept of the unitary atomic scattering factor best applies. Now, equation (1) can be written as

$$f_{0j}/N_j = \exp \left( \sum_{k=1}^n \alpha_{jk} x^k \right) \quad (5)$$

where the sub-index  $j$  has been added to designate the atomic species. Substituting equation (5) into (4) yields

$$\hat{f}_0 \approx \exp \left[ (1/P) \sum_{j=1}^P \sum_{k=1}^n \alpha_{jk} x^k \right] = \exp \left( \sum_{k=1}^n \beta_k x^k \right) \quad (6)$$

where

$$\beta_k = (1/P) \sum_{j=1}^P \alpha_{jk}; \quad \beta_0 = 0. \quad (7)$$

Thus,  $\hat{f}_0$  can be simply and rapidly calculated using equation (6), an expression of the same form as (1). The  $\beta_k$ 's, the new least-squares parameters, are derived by taking the arithmetic mean of the corresponding least-

squares parameters of the contents of the unit cell.  $\hat{f}_0$ , which includes temperature motion, can also be directly calculated using equation (6) if the  $\alpha_{j2}$ 's are first modified by subtraction of the natural temperature factors, the  $B_j$ 's. Further, the quantity

$$\sum_{j=1}^P f_{0j}^2,$$

useful in statistical work, can be calculated with sufficient accuracy when the atoms in the structure do not differ greatly in atomic number by a slight modification in the above procedure. With the usual assumption,  $f_{0j} \approx \hat{f}_0 N_j$ , we obtain

$$\sum_{j=1}^P f_{0j}^2 \approx \hat{f}_0^2 \sum_{j=1}^P N_j^2 \approx \left( \sum_{j=1}^P N_j^2 \right) \exp \left( 2 \sum_{k=1}^n \beta_k x^k \right) \quad (8)$$

We therefore have a very convenient and simple computational method for sharpening Patterson and Fourier syntheses, calculating unitary structure factors for use in inequalities, and determining absolute scaling constants and natural temperature factors by Wilson's (1942) statistical method.

#### Structure refinement

The very accurate interpolated  $f_0$  values obtained from the unique polynomial coefficients of Table 2 may be used for structure factor calculation in the final stages of structure refinement. We have computed tables of  $f_0$  values with these coefficients for the Cu  $K\alpha$  radiation range at intervals of 0.001 in  $\sin^2 \theta$  (0.000–1.000). In

computation, it is convenient to introduce the wavelength by the use of modified coefficients,  $\alpha'_k$ , where  $\alpha'_k = \alpha_k/\lambda^k$  so that the independent variable becomes  $\sin \theta$ .

Our tables also include  $f_0$  values corrected for dispersion with the data of Dauben & Templeton (1955).

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**On the structure of evaporated carbon films.** By JON GJØNNES, *Central Institute for Industrial Research, Oslo, Norway*

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During an investigation by the present author on multiple scattering effects in electron diffraction, several diffractograms were taken of evaporated carbon films in the thickness range 100–600 Å. It is the purpose of this note to discuss the radial distribution curves which were obtained from these diffractograms after performing correction for multiple scattering as described in a recent paper (Gjønnnes, 1959). The diffractograms consisted of a series of diffuse halos with no signs of the graphite crystallites occasionally observed by Cosslett & Cosslett (1959) from similar specimens. Apart from multiple scattering effects no variations with film thickness were observed in the diffractograms. The  $s(4\pi \sin \theta/\lambda)$  values for the halos were found to correspond closely to those reported by Kakinoki *et al.* (1957).

The atomic radial distribution curve shown in Fig. 1 was calculated from intensity data in the region  $s = 1\text{--}20 \text{ \AA}^{-1}$ . Normalization and subtraction of back-ground was carried out according to the procedure extensively used by Almenningen *et al.* (1955) in gas investigations.

As the intensity at small angles was neglected, the calculated radial distribution corresponds to the deviations from the even distribution (see e.g. Klug & Alexander, 1954). To obtain the total atomic distribution function one must therefore read the ordinate above the straight line in Fig. 1 corresponding to *minus* the normalized even distribution. The  $r$ -values of the peaks in the  $\sigma/r$ -curve are tabulated in the first column of Table 1 together with the peak areas found by decomposition and integration of  $\sigma(r)$ . The values in the next two columns are calculated for a single graphite layer with bond length equal to the observed nearest neighbor distance, *viz.* 1.45 Å. By comparison it is at once seen that the observed interatomic distances do not fit well with a planar hexagonal layer, and it is further noticed that the observed nearest neighbor distance is appreciably greater than that found in graphite (1.42 Å).

Attempts to account for those discrepancies by introducing variations in bond angle and deviations from planarity indicate the latter to be considerable. It thus seems reasonable to seek an interpretation of the experimental radial distribution by a three-dimensional network like those previously suggested by Gilson *et al.* (1946) or Kakinoki *et al.* (1957). The distances and weights tabulated in the last two columns of Table 1 correspond to the model proposed by Gilson *et al.* (1946). This structure consists essentially of a mixture of 6-rings and staggered 8-rings, the atomic arrangement around each 8-ring being similar to that found for tetraphenylene by Karle & Brockway (1944). The C–C bonds within and between the 6-rings were taken to be 1.40 and 1.52 Å respectively and all C–C–C angles were set equal to 120°, in close agreement with the reported values for tetraphenylene.

The agreement between the latter model and the observed radial distribution may be judged from Table 1. As a further illustration we have calculated  $\sigma/r$ -curves for this model and a turbostratic packing (see Biscoe & Warren (1942) or Franklin (1951)) of graphite layers, with  $r = 1.45 \text{ \AA}$  and an interlayer distance of 3.40 Å.

Table 1. Observed and calculated interatomic distances

Observed		Graphite layer		Three-dimensional network		
$r$ (Å)	No. of atoms	$r$ (Å)	No. of atoms	$r$ (Å)	Average	No. of atoms
1.45	2.9	(1.45)	3	{ 1.40 1.52	1.44	{ 2 1
2.49	7	2.51	6	{ 2.42 2.53	2.49	{ 2 4
3.1	7	2.90	3	{ 2.80 2.92	3.09	{ 1 2
3.74	12–14	3.84	6	{ 3.24 3.58 3.82	3.77	{ 4 2 8
4.52		4.35	6	{ 4.32 4.55 4.75		{ 10 6 7
4.95		{ 5.02 5.22	{ 6 6		{ 5.00 5.17	{ 5 14