Analytical Approximations for Coherent and Incoherent Atomic Scattering Factors

By Shuzo SHIBATA

Department of Chemistry, Faculty of Science, Shizuoka University, Oiwa, Shizuoka

(Received November 29, 1965)

For the analysis of gas electron-diffraction data by the use of an electronic computer, analytical approximations[1] for coherent and incoherent atomic scattering factors are useful in order to decrease the amount of input data and to obtain their values for arbitrary scattering angles by smooth interpolation. A simple analytical function, $\exp(\sum a_n q^n)$, was found to be a good approximation for the coherent and incoherent atomic scattering factors. Here q is the scattering variable defined by $40\sin(\theta/2)/\lambda$, where θ is the scattering angle and λ is the wavelength of the incident X-rays or electrons. Such an expression was used by Silverman and Simonsen[2] for atomic scattering factors for an X-ray analysis. In their work, however, the values of the scattering variable, q, were limited to within 50. The q values usually convered by the experimental data of gas electron diffraction, however, range from 10 to 100. The present calculation of the analytical constants has, therefore, been carried out to cover this range of the scattering variable. The scattering factors given by Viervoll and Ögrim[3] were adopted in the present calculation, because no other scattering factors[4] calculated thus far extend to sufficiently large scattering angles.*1

The parameters of the polynomials were determined by a least-square method by minimizing $\sum_i(\ln f_{0i}-\ln f_i)^2$, where f_0 is the theoretical value and f is the calculated value. The evaluation was straightforward because the parameters were taken as linear. The function was tested mainly with polynomials of the fifth, sixth and seventh degrees. The standard deviation, σ, given by $[\sum_i(f_{0i}-f_i)^2/N]^{1/2}$, was calculated in each case. Here N is the number of the values fitted. The sixth-degree polynomial exponent gave a σ value smaller than that for the fifth-degree, whereas the polynomial exponent of a degree higher than the sixth did not give a much better fit. A typical case is presented in Table I. The parameters obtained are tabulated in Table II, with their standard deviations for twenty-three atoms from hydrogen to copper. Theoretical values below 9.55 in q were not used for the fitting, since the values in this range are not needed for usual analyses of gas electron diffraction.*2 Therefore, another set of parameters should be used if coherent scattering factors for smaller q values are required. This latter set was obtained by fitting thirty theoretical values of Viervoll and Ögrim*3, beginning with 3.18 in q, by a sixth-degree polynomial exponent. The standard deviation was somewhat larger. Table III shows several different sets of analytical constants for the coherent atomic scattering factor of carbon with varying minimum q values and varying numbers of the theoretical values fitted.

The incoherent scattering factor, $S(v)$, calculated by Bewilogua[7] was approximated by an analytical function, $1\text{-}\exp(\sum b_n v^n)$, where $v=0.0553\cdot Z^{-2/3}\cdot q$ and Z is the atomic number. The exponent of a fifth-degree polynomial was found to be sufficient to reproduce the theoretical values with a good accuracy over the entire range of v. The sets of parameters are tabulated in Table IV for various degrees of polynomial exponents. The incoherent scattering factors approximated by the fifth-degree polynomial exponent are compared in Table V with those calculated by Bewilogua.

1) For example, R. A. Bonham and L. S. Bartell, *J. Chem. Phys.*, **31**, 702 (1959).

2) J. N. Silverman and S. H. Simonsen, *Acta Cryst.*, **13**, 50 (1960).

3) H. Viervoll and O. Ögrim, ibid., **2**, 277 (1949).

4) "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham (1962), p. 201.

*1 One exception is the atomic scattering factor calculated by Hanson et al.[5] from the Hartree-Fock-Slater wave function, but Viervoll and Ögrim's factors agree better with the absolute values of complex atomic scattering factors,[4] $|f|$, than Hanson's factors.

*2 Another reason for this was that the scattering factors in this region may be uncertain because of the exchange effect of electrons.

*3 It is desirable, however, to use other theoretical scattering factors obtained with reference to the exchange effect. For example, by the use of the scattering factor of carbon by Berghuis et al.,[6] the fit with a sixth-degree polynomial exponent resulted in the standard deviation of 0.013. Silverman and Simonsen, however, obtained 0.095 for the standard deviation from the same fit with a fixed coefficient, a_0.

5) H. P. Hanson, F. Herman, J. D. Lea and S. Skillman, *Acta Cryst.*, **17**, 1040 (1964).

6) J. Berghuis, I. M. Haanappel, M. Potters, B. O. Loopstra, C. H. MacGillavry and A. L. Veenendaal, ibid., **8**, 478 (1955).

7) L. Bewilogua, *Physik. Z.*, **32**, 740 (1931); R. F. Pohler and H. P. Hanson, *J. Chem. Phys.*, **42**, 2347 (1965).

TABLE I. COEFFICIENTS OF nTH-DEGREE POLYNOMIALS FOR THE COHERENT ATOMIC SCATTERING FACTOR OF CARBON ($N=28$)

n	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	σ
5	1.8433−00*	−1.3932−01	5.4999−03	−1.1420−04	1.0676−06	−3.7104−09			0.021
6	2.1970−00	−2.0823−01	1.0283−02	−2.7020−04	3.6524−06	−2.4757−08	6.6793−11		0.011
7	2.4910−00	−2.7565−01	1.6082−02	−5.1739−04	9.4019−06	−9.8896−08	5.6394−10	−1.3512−12	0.007

* The last number repnesents a negative exponent of ten.

TABLE II. COEFFICIENTS OF SIXTH-DEGREE POLYNOMIALS FOR COHERENT ATOMIC SCATTERING FACTORS ($N=28$)

	a_0	a_1	a_2	a_3	a_4	a_5	a_6	σ
H*	−3.2611−01	5.4004−02	−1.9266−02	7.8699−04	−1.4974−05	1.3675−07	4.7794−10	0.001
Li	8.4174−01	−3.3521−02	4.9715−04	−6.8484−05	1.7129−06	−1.6384−08	5.4439−08	0.005
Be	7.3021−01	−5.0064−03	−1.0412−03	1.6923−05	−2.2814−07	2.0500−09	−7.0528−12	0.007
B	1.6535−00	−1.6119−01	9.1676−03	−2.8670−04	4.4760−06	−3.4297−08	1.0272−10	0.005
C	2.1970−00	−2.0823−01	1.0283−02	−2.7020−04	3.6524−06	−2.4757−08	6.6793−11	0.011
N	2.8661−00	−2.5134−01	1.0868−02	−2.5204−04	3.1174−06	−1.9902−08	5.1786−11	0.010
O	2.9909−00	−2.0115−01	6.4790−03	−1.1203−04	1.0062−06	−4.4423−09	7.2910−12	0.014
F	2.9959−00	−1.6678−01	3.8705−03	−3.2369−05	−1.7407−07	4.1810−09	−1.7718−11	0.023
Na	2.3403−00	7.0460−03	−5.7283−03	2.0797−04	−3.3038−06	2.4970−08	−7.3365−11	0.017
Mg	2.0420−00	6.0336−02	−7.9086−03	2.4955−04	−3.7272−06	2.7255−08	−7.8583−11	0.008
Al	2.0656−00	5.2360−02	−6.2717−03	1.7894−04	−2.4310−06	1.6253−08	−4.3016−11	0.026
Si	2.1408−00	3.4000−02	−4.1630−03	9.9729−05	−1.0707−06	5.1857−09	−8.3662−12	0.021
P	2.3697−00	−1.0998−02	−5.7333−04	−1.7808−05	7.9342−07	−9.1204−09	3.4265−11	0.031
S	2.7052−00	−6.8324−02	3.2356−03	−1.2704−04	2.3420−06	−1.9856−08	6.3385−11	0.033
Cl	3.0847−00	−1.3040−01	7.0695−03	−2.3133−04	3.7560−06	−2.9283−08	8.8069−11	0.032
K	3.4737−00	−1.5181−01	6.5707−03	−1.6360−04	2.0654−06	−1.2648−08	2.9892−11	0.020
Ca	3.4323−00	−1.2669−01	4.5825−03	−9.8072−05	1.0585−06	−5.4341−09	1.0398−11	0.029
Cr	3.4279−00	−8.4891−02	1.4187−03	2.6254−06	−4.4222−07	5.1776−09	1.8620−11	0.027
Mn	3.3939−00	−6.9591−02	4.9198−04	2.6688−05	−7.4449−07	7.0212−09	−2.3053−11	0.028
Fe	3.3823−00	−5.4476−02	−5.2283−04	5.5036−05	−1.1352−06	9.7154−09	−3.0558−11	0.021
Co	3.3874−00	−4.2935−02	−1.2734−03	7.4851−05	−1.3906−06	1.1348−08	−3.4753−11	0.025
Ni	3.3937−00	−3.3398−02	−1.7302−03	8.1794−05	−1.4025−06	1.0862−08	−3.1949−11	0.014
Cu	3.4643−00	−3.0981−02	−1.7937−03	7.7501−05	−1.2464−06	9.1136−09	−2.5368−11	0.022

* $N=23$

TABLE III. COEFFICIENTS OF POLYNOMIALS FITTED WITH N THEORETICAL VALUES FOR THE COHERENT ATOMIC SCATTERING FACTOR OF CARBON ($n=6$)

N	a_0	a_1	a_2	a_3	a_4	a_5	a_6	σ	Min. of q
31	1.8724−00	−1.2645−01	3.9282−03	−5.1303−05	−7.7045−08	6.0468−09	−3.1649−11	0.143	0.000
30	2.1996−00	−2.0492−01	9.9091−03	−2.5529−04	3.3787−06	−2.2393−08	5.9015−11	0.030	3.183
29	2.3437−00	−2.3317−01	1.1830−02	−3.1624−04	4.3608−06	−3.0185−08	8.3172−11	0.012	6.366
28	2.1970−00	−2.0823−01	1.0283−02	−2.7020−04	3.6524−06	−2.4757−08	6.6793−11	0.011	9.549
27	1.8072−00	−1.4880−01	6.8739−03	−1.7434−04	2.2395−06	−1.4286−08	3.6023−11	0.006	12.732

TABLE IV. COEFFICIENTS OF nTH-DEGREE POLYNOMIALS FOR INCOHERENT SCATTERING FACTORS

n	b_0	b_1	b_2	b_3	b_4	b_5	b_6	b_7	σ
2	−1.2400−1	−4.9727−0	1.8619−0						0.036
3	−5.5375−2	−6.1628−0	5.0333−0	−2.1275−0					0.018
4	−2.4933−2	−7.1168−0	9.7444−0	−9.6371−0	3.7490−0				0.009
5	−7.5548−3	−8.0228−0	1.7051+1	−3.0220+1	2.7384+1	−9.4823−0			0.003
6	−4.1362−3	−8.3308−0	2.0873+1	−4.7045+1	6.0497+1	−3.9346+1	1.0060+1		0.002
7	−9.2425−4	−8.8929−0	3.0952+1	−1.1073+2	2.4845+2	−3.2171+2	2.1938+2	−6.0752+1	0.001

TABLE V. COMPARISON BETWEEN BEWILOGUA'S INCOHERENT SCATTERING FACTORS S_0 AND LEAST-SQUARES VALUES S CALCULATED WITH FIFTH-DEGREE POLYNOMIAL EXPONENT

v	S_0	S	v	S_0	S	v	S_0	S
0.00	0.000	0.007	0.3	0.776	0.776	0.7	0.929	0.929
0.05	0.319	0.310	0.4	0.839	0.838	0.8	0.944	0.944
0.10	0.486	0.487	0.5	0.880	0.880	0.9	0.954	0.954
0.20	0.674	0.677	0.6	0.909	0.909	1.0	0.963	0.963