

SHORT COMMUNICATIONS

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A note on the values of the ratio of the imaginary to the real part of the atomic scattering factors for the X-ray $K\alpha_1$ and $K\beta_1$ radiations.* By V. PARTHASARATHI and S. PARTHASARATHY, *Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras-600025, India*

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The values of the ratio (k) of the imaginary to the total real part of the atomic scattering factor are obtained for atoms with $Z=10$ to 98 for the $K\alpha_1$ and $K\beta_1$ radiations of Cr, Fe, Cu, Mo and Ag. Numerical tables contain the value of k corresponding to the forward direction (denoted by k_0) and the average values of k for the ranges $\theta=0$ to 50° and $\theta=0$ to 90° (denoted by \bar{k}_{50° and \bar{k}_{90° , respectively).

The probability distributions of quantities such as the normalized Bijvoet differences x and Δ (Parthasarathy & Srinivasan, 1964), Bijvoet ratio δ (Parthasarathy, 1967; Parthasarathy & Parthasarathi, 1973), anomalous phase angle α_A (Parthasarathy, Sabesan & Venkatesan, 1970), and the phase angle error θ (Parthasarathy, 1965) are found to depend on the parameter $k = [A f''/(f_0 + A f'')] \dagger$ which is the ratio of the imaginary to the total real part of the atomic scattering factor of the anomalously scattering atoms in the unit cell. Further it can be seen (see the above references) that the distributions of x , Δ , δ , α_A and θ are more sensitive to variations in the value of k than in the other parameter (*i.e.* σ_1^2) defining the relevant distributions. It is therefore useful for the purpose of ready reference, to tabulate the values of k for various atoms for different X-radiations.

Though the value of the imaginary part $A f''$ (which owes its existence to the inner-most electrons) of an atom for a given wavelength could be taken to be practically constant for various values of the Bragg angle θ , the quantity k will be a monotonically increasing function of $(\sin \theta)/\lambda$ (abbreviated as s), owing to the marked fall of the atomic scattering factor f_0 with increasing s . The average values of k over the various values of s for a few atoms for Cu $K\alpha$ and Mo $K\alpha$ radiations have been calculated by Parthasarathy (1967) and it can be seen that the average value \bar{k} (denoted hereafter by \bar{k}) of an atom for a given wavelength is significantly different from the value corresponding to the forward direction (denoted by k_0). Since, for the application of the theoretical distributions of x , Δ , δ , α_A and θ the value of \bar{k} is more important than that of k_0 , we shall evaluate \bar{k} for atoms with $Z=10$ to $Z=98$. In some actual crystals, because of thermal vibrations, the reflexions for which θ is large (say, $\theta>50^\circ$) may be too weak to be measured (see Hall & Maslen, 1965). It would therefore be useful to have the values of \bar{k} for the range $\theta=0$ to 50° as well. Since the

Table 1. Values (%) of the ratio of the imaginary to the total real part of the atomic scattering factors for the $K\alpha_1$ radiations of Cr, Fe, Cu, Mo and Ag

ATOM	Cr $K\alpha_1$			Fe $K\alpha_1$			Cu $K\alpha_1$			Mo $K\alpha_1$			Ag $K\alpha_1$				
	k_0	\bar{k}_{50°	\bar{k}_{90°														
He	1.0	2.0	3.2	2.1	2.1	2.2	0.4	2.2	2.2	1.0	0.8	1.0	0.1	0.6	0.7		
H	2.1	3.5	5.0	2.5	2.5	2.5	1.1	2.1	2.1	2.1	1.0	1.0	0.2	0.4	0.5		
Li	2.1	3.5	5.0	2.5	2.5	2.5	1.1	2.1	2.1	2.1	1.0	1.0	0.2	0.4	0.5		
Si	7.0	8.2	9.2	5.6	5.8	5.6	2.3	4.2	5.0	5.8	1.9	2.7	0.3	1.6	1.8		
P	9.0	10.2	11.2	6.2	6.5	6.2	3.0	5.0	5.8	6.2	1.7	2.7	0.3	1.6	1.7		
Cl	10.9	12.0	12.5	7.2	7.5	7.2	3.0	5.0	5.8	6.2	1.7	2.7	0.3	1.6	1.7		
Ar	8.2	9.7	10.7	6.0	6.3	6.0	2.0	3.7	4.0	4.8	1.5	2.5	0.3	1.6	1.7		
Ca	12.7	13.9	15.0	8.7	9.5	10.3	3.5	5.5	6.2	7.0	2.0	2.8	0.3	1.6	1.7		
Ti	12.1	13.6	15.2	9.0	10.0	10.5	3.5	5.5	6.2	7.0	2.0	2.8	0.3	1.6	1.7		
V	2.4	3.9	4.9	2.5	2.5	2.5	0.9	1.7	2.0	2.9	1.0	6.4	2.9	1.3	6.5		
Cr	12.7	13.9	15.0	9.0	10.0	10.5	3.5	5.5	6.2	7.0	2.0	2.8	0.3	1.6	1.7		
W	12.1	13.6	15.2	9.0	10.0	10.5	3.5	5.5	6.2	7.0	2.0	2.8	0.3	1.6	1.7		
Fe	3.1	4.5	5.2	2.5	2.5	2.5	0.7	1.5	1.5	2.0	0.9	9.3	11.7	0.9	8.7		
Co	12.7	13.9	15.0	9.0	10.0	10.5	3.5	5.5	6.2	7.0	2.0	2.8	0.3	1.6	1.7		
Ni	5.3	6.1	7.0	2.9	3.1	3.1	2.0	3.8	4.0	5.0	1.9	12.7	15.5	2.0	9.9		
Cu	5.2	6.7	6.8	2.5	2.7	2.7	2.0	3.8	4.0	5.0	1.9	12.7	15.5	2.0	9.9		
Sn	5.3	6.9	7.1	2.9	3.5	3.5	2.0	3.8	4.0	5.0	1.9	12.7	15.5	2.0	9.9		
Ge	7.3	7.6	8.6	4.7	5.2	5.2	2.5	3.8	4.0	5.0	1.9	12.7	15.5	2.0	9.9		
Se	6.3	9.2	10.2	5.1	7.1	8.5	3.5	5.5	6.2	6.8	20.2	26.8	4.3	16.6	21.1		
Br	10.0	10.0	11.7	6.0	6.1	6.1	2.5	3.8	4.0	5.0	1.9	21.5	31.1	1.9	16.1	25.0	
Rb	8.3	11.3	12.2	6.5	9.5	10.8	3.5	7.2	8.5	9.5	1.9	25.2	33.0	5.0	16.3	27.0	
Y	12.1	13.6	15.2	7.2	10.5	13.0	3.5	7.2	8.5	9.5	1.9	25.2	33.0	5.0	16.3	27.0	
Zr	11.3	13.1	14.8	8.5	12.1	15.0	3.5	7.2	8.5	9.5	1.9	25.2	33.0	5.0	16.3	27.0	
Tc	13.7	14.7	17.0	9.0	10.3	11.1	3.5	7.2	8.5	9.5	1.9	25.2	33.0	5.0	16.3	27.0	
Ru	13.7	14.7	17.0	9.0	10.3	11.1	3.5	7.2	8.5	9.5	1.9	25.2	33.0	5.0	16.3	27.0	
Po	16.7	22.5	23.5	12.0	18.2	20.9	8.0	13.5	16.2	18.5	2.5	6.5	8.1	1.5	5.8	6.5	
Te	24.5	26.8	28.1	12.0	19.5	23.0	9.5	15.5	16.5	18.5	2.5	6.5	8.1	1.5	5.8	6.5	
In	27.5	31.1	31.1	15.2	21.2	25.8	10.3	16.4	19.6	21.7	2.5	7.9	9.3	1.5	6.1	8.3	
Sr	31.3	31.9	36.1	17.2	24.2	28.4	12.6	18.4	21.7	25.3	2.5	8.5	10.3	2.0	6.7	9.0	
Tl	25.1	34.7	35.1	18.3	26.5	30.2	12.3	18.7	23.0	25.3	2.5	8.5	10.3	2.0	7.1	9.3	
Al	26.1	37.3	37.3	18.3	26.5	30.2	12.3	18.7	23.0	25.3	2.5	8.5	10.3	2.0	7.1	9.3	
Ge	32.6	37.3	37.3	20.7	30.1	35.1	13.8	21.2	25.8	28.5	2.5	9.8	12.0	2.5	7.6	10.2	
Cs	29.2	35.0	50.0	22.0	32.9	37.5	14.0	21.5	25.2	28.0	2.5	10.8	12.7	2.5	8.6	10.2	
La	7.0	11.9	13.9	25.7	35.1	45.6	16.5	26.5	30.8	43.3	11.5	14.1	2.9	9.3	11.7		
Ce	7.0	11.9	13.9	25.7	35.1	45.6	17.5	27.5	32.7	43.3	11.5	14.1	2.9	10.3	12.9		
Ho	8.0	11.7	13.3	20.2	31.1	37.6	19.3	31.1	36.8	45.3	13.3	16.8	5.0	10.8	15.5		
Eu	9.0	12.8	16.4	23.0	33.0	37.6	20.5	33.0	39.2	45.3	13.3	16.8	5.0	11.5	16.1		
Gd	9.0	12.8	16.4	23.0	33.0	37.6	21.5	33.0	39.2	45.3	13.3	16.8	5.0	11.5	16.1		
Dy	10.0	16.1	18.7	24.8	32.0	37.6	17.5	29.3	35.9	45.3	17.5	21.7	5.5	13.6	17.0		
Er	12.2	16.1	16.5	24.8	32.0	37.6	18.1	30.1	37.7	45.3	17.5	21.7	5.5	13.6	17.0		
Tb	12.2	16.5	17.5	9.5	13.1	15.0	6.0	11.1	13.5	17.5	18.7	25.7	5.5	15.5	21.1		
Tu	12.1	16.1	16.7	10.2	14.0	16.0	13.9	17.1	19.5	21.6	26.8	5.5	17.4	27.1			
Lu	12.1	16.1	16.7	10.2	14.0	16.0	13.9	17.1	19.5	21.6	26.8	5.5	17.4	27.1			
Wf	12.0	17.5	19.5	10.7	14.5	16.5	13.6	17.7	19.6	21.8	27.9	5.5	17.4	27.1			
Ta	12.0	17.5	19.5	10.7	14.5	16.5	13.6	17.7	19.6	21.8	27.9	5.5	17.4	27.1			
W	12.0	17.5	19.5	10.7	14.5	16.5	13.6	17.7	19.6	21.8	27.9	5.5	17.4	27.1			
Re	12.5	19.7	21.8	12.0	16.3	18.6	8.5	12.9	15.0	19.5	21.2	27.1	5.5	17.4	27.1		
Os	12.5	19.7	21.8	12.0	16.3	18.6	8.5	12.9	15.0	19.5	21.2	27.1	5.5	17.4	27.1		
Pt	17.6	22.1	26.1	13.5	18.2	20.5	9.5	14.3	16.6	18.6	21.1	27.1	35.7	7.9	22.3	29.2	
Al	21.7	25.4	27.7	13.5	18.2	20.5	10.0	17.1	21.7	23.5	22.5	29.2	35.7	11.1	33.0	39.6	
Ag	18.1	23.1	26.4	18.5	19.6	22.0	10.7	15.3	17.7	17.0	20.5	28.5	33.1	8.0	25.8	31.6	
Mg	18.1	23.1	26.4	18.5	19.6	22.0	10.7	15.3	17.7	17.0	20.5	28.5	33.1	8.0	25.8	31.6	
Li	19.5	24.8	27.7	15.1	20.3	22.8	10.6	15.8	18.3	17.0	20.5	28.5	33.1	8.0	25.8	31.6	
Tl	20.5	24.8	27.7	15.1	20.3	22.8	10.6	15.8	18.3	17.0	20.5	28.5	33.1	8.0	25.8	31.6	
Bi	21.1	26.8	29.6	16.2	21.0	24.5	11.1	17.0	19.6	19.5	23.6	33.6	34.3	9.0	26.3	35.1	
Po	21.9	26.0	30.9	16.8	21.7	25.5	11.8	17.6	20.2	21.2	33.8	35.8	43.5	9.5	27.1	34.9	
At	22.4	27.1	30.9	17.3	22.0	25.8	12.3	18.1	21.6	22.7	34.3	35.8	43.5	10.0	27.6	35.1	
Ar	23.4	30.5	33.5	18.1	24.3	27.6	12.7	18.9	21.6	23.5	34.5	36.7	45.1	10.0	29.3	39.5	
Br	24.5	31.0	34.8	19.1	25.8	28.5	13.1	19.7	22.1	24.1	34.5	36.7	45.1	10.3	31.6	42.7	
Ca	24.6	31.4	34.8	20.1	27.8	30.6	13.0	19.6	22.9	24.1	34.5	36.7	45.1	10.3	31.6	42.7	
AC	26.4	34.5	38.0	20.1	27.8	30.6	13.0	19.6	22.9	24.1	34.5	36.7	45.1	11.1	33.0	42.6	
Fe	27.7	34.7	37.7	21.5	28.9	32.0	13.0	19.7	23.5	25.3	34.5	36.7	45.1	12.0	34.5	43.6	
PA	24.5	37.1	39.5	22.2	30.3	34.1	13.5	23.5	26.4	31.9	33.8	35.9	37.5	38.7	13.7	34.5	43.6
U	24.5	37.1	39.5	22.2	30.3	34.1	13.5	23.5	26.4	31.9	33.8	35.9	37.5	38.7	13.7	34.5	43.6
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quantity $\Delta f''$ for an atom depends explicitly on the wavelength used, the value \bar{k} also will differ for different wavelengths. We shall hence tabulate the value of k_0 , k_{500} and \bar{k}_{900}^* for the $K\alpha_1$ and $K\beta_1$ radiations of Cr, Fe, Cu, Mo and Ag.

The value of \bar{k} for a given range of s , say $s=0$ to s_1 , can be obtained by the following procedure. Imagine the reciprocal space to be divided into a number of thin spherical shells and consider one such elementary shell of radius $H (= 2s)$ and thickness dH . The value of k in this shell can

* Here \bar{k}_{50° denotes the average value of k for the range $\theta=0$ to 50° while \bar{k}_{90° denotes that for the entire range of θ , viz., $\theta=0$ to 90° .

Table 2. Values (%) of the ratio of the imaginary to the total real part of the atomic scattering factors for the $K\beta_1$ radiations of Cr, Fe, Cu, Mo and Ag

ATOM	CrK _β			FeK _β			CuK _β			MoK _β			AgK _β		
	K _o	K _o '	E _o '	K _o	K _o '	E _o '	K _o	K _o '	E _o '	K _o	K _o '	E _o '	K _o	K _o '	E _o '
10 NE	2.5	3.4	3.0	1.5	2.1	1.7	0.8	1.7	2.4	0.2	1.1	1.3	0.1	0.7	0.4
11 O	2.5	3.1	3.7	1.5	2.6	4.0	1.5	2.2	3.6	0.3	1.4	0.2	0.3	1.2	2.6
12 MA	2.7	4.1	4.8	1.5	2.5	4.0	1.5	2.3	3.6	0.3	1.7	2.0	0.2	1.2	2.6
13 AI	2.7	3.7	4.5	1.5	2.5	4.1	2.1	4.1	5.0	0.6	2.5	3.6	0.1	0.7	0.4
14 SI	2.7	3.7	4.5	1.5	2.5	4.1	2.1	4.1	5.0	0.6	2.5	3.6	0.1	0.7	0.4
15 S	3.0	8.0	8.1	5.7	6.5	7.4	7.5	8.3	8.8	0.7	2.4	8.0	0.5	3.7	3.7
16 CL	7.0	11.5	13.2	5.2	9.3	10.7	3.0	7.1	8.2	0.9	3.5	9.0	0.6	6.6	6.6
17 AR	8.2	13.5	15.8	6.1	10.3	12.6	5.1	8.1	9.4	1.1	4.0	5.6	0.7	13.2	13.2
18 CI	11.1	18.0	21.2	4.5	13.6	17.3	5.5	11.3	12.9	1.5	3.5	8.9	1.0	10.0	10.0
19 TN	13.0	20.0	24.7	8.5	16.5	19.8	6.9	12.9	15.4	1.7	5.5	7.6	1.1	20.0	20.0
20 CA	13.5	23.5	27.5	10.5	21.5	25.1	9.0	16.1	19.6	2.1	7.3	9.1	1.4	23.5	23.5
21 TI	13.5	23.5	27.5	10.5	21.5	25.1	9.0	16.1	19.6	2.1	7.3	9.1	1.4	23.5	23.5
22 Y	13.5	23.5	27.5	10.5	21.5	25.1	9.0	16.1	19.6	2.1	7.3	9.1	1.4	23.5	23.5
23 CR	13.5	23.5	27.5	10.5	21.5	25.1	9.0	16.1	19.6	2.1	7.3	9.1	1.4	23.5	23.5
24 FE	3.0	5.2	6.2	3.0	5.1	6.2	11.3	21.0	27.7	2.9	10.1	12.3	1.9	10.1	10.1
25 CO	3.0	5.2	6.5	2.0	5.0	6.2	12.7	26.6	31.1	3.2	11.1	15.8	2.1	8.2	8.2
26 CU	3.0	5.2	6.7	3.0	5.1	6.2	2.6	5.6	6.1	1.5	15.5	16.3	1.4	16.5	16.5
27 ZN	3.0	5.2	6.7	3.0	5.1	6.2	2.6	5.6	6.1	1.5	15.5	16.3	1.4	16.5	16.5
28 GE	3.0	5.2	6.7	3.0	5.1	6.2	5.0	11.3	12.7	5.0	17.1	21.1	1.4	15.1	15.1
29 AS	3.0	5.2	6.7	3.0	5.1	6.2	5.2	11.6	7.0	5.5	18.5	23.5	1.4	15.0	15.0
30 BR	6.6	9.3	10.5	5.1	7.1	9.1	5.7	6.5	7.8	6.3	21.1	27.6	4.7	15.7	21.4
31 SH	6.6	9.3	10.5	5.1	7.1	9.1	4.0	6.5	8.8	6.3	21.1	27.6	4.7	15.7	21.4
32 SR	6.6	9.3	10.5	5.1	7.1	9.1	4.7	10.1	9.5	7.9	26.1	35.8	2.1	22.1	27.5
33 IR	9.3	12.6	13.5	7.0	11.0	13.5	5.5	9.5	10.7	9.3	21.3	35.3	8.0	22.3	32.3
34 HS	10.2	14.6	15.5	8.0	12.1	14.0	5.7	8.4	11.5	10.3	36.0	55.8	8.4	25.9	35.0
35 TC	10.2	14.6	15.5	8.0	12.1	14.0	6.0	8.4	11.2	2.1	21.1	31.1	9.1	25.9	35.0
36 RU	12.2	17.3	18.7	9.5	14.5	16.4	6.7	11.7	13.6	2.7	7.1	10.0	7.9	32.1	36.0
37 PO	13.7	19.7	22.0	10.5	16.5	18.6	7.5	12.5	15.2	2.5	7.4	10.1	10.3	32.1	36.0
38 AG	14.6	20.3	23.1	11.2	16.9	19.7	7.9	13.6	16.1	2.5	7.5	10.3	1.9	18.1	18.1
39 SN	14.6	20.3	23.1	11.2	16.9	19.7	8.1	13.6	17.9	2.4	7.5	10.3	1.9	18.1	18.1
40 SH	14.6	20.3	23.1	11.2	16.9	19.7	9.5	13.6	18.9	3.0	8.1	11.3	2.1	20.1	21.4
41 TE	19.7	28.0	32.0	18.1	21.1	25.0	10.4	17.6	20.9	5.3	9.7	12.2	2.3	8.7	12.7
42 I	21.1	30.2	35.4	15.5	23.9	27.6	11.0	18.6	22.0	5.5	10.4	17.7	4.9	8.9	12.7
43 CS	24.7	36.7	38.4	17.9	25.7	31.6	12.3	20.8	26.6	5.9	11.2	13.9	2.7	9.5	33.1
44 BS	22.7	35.1	35.4	19.0	29.5	33.5	11.0	22.1	27.3	4.1	11.1	14.5	2.9	12.5	26.5
45 LA	18.5	24.0	32.4	21.1	33.6	39.2	14.5	20.8	38.9	4.5	17.8	15.8	3.2	11.1	18.4
46 NO	7.5	10.8	12.5	11.6	13.1	14.1	15.5	20.6	30.5	5.0	14.5	16.8	3.5	11.5	18.4
47 EU	8.0	11.1	12.5	7.7	10.1	13.5	15.5	21.7	32.7	5.0	14.5	16.8	3.5	11.5	18.4
48 GD	8.3	13.5	15.2	6.3	10.1	12.9	19.8	33.6	39.7	5.6	16.0	19.8	4.0	15.7	17.2
49 DT	9.0	12.1	15.7	7.1	10.5	12.9	17.8	31.1	37.2	6.1	20.5	23.5	5.5	16.5	17.2
50 TH	9.0	12.1	15.7	7.1	10.5	12.9	17.8	31.1	37.2	6.1	20.5	23.5	5.5	16.5	17.2
51 TR	9.7	12.9	19.4	7.6	11.0	12.8	17.7	25.3	31.2	4.8	21.4	25.7	4.0	16.5	20.3
52 TS	9.9	13.5	15.4	7.8	11.2	15.0	6.2	11.0	15.9	7.6	13.5	24.5	5.5	16.5	21.0
53 HF	10.6	14.0	15.4	8.3	11.8	15.6	6.1	10.0	12.3	7.3	20.5	26.7	5.5	17.7	22.5
54 TA	11.0	14.5	16.3	8.6	12.5	14.0	6.3	12.0	12.3	7.4	21.1	27.1	5.8	18.6	23.2
55 RE	12.0	15.1	17.7	9.3	13.2	15.1	6.7	13.0	15.8	8.1	22.5	29.0	5.5	19.5	24.3
56 DS	12.5	15.5	18.3	9.7	13.6	15.8	6.9	11.1	15.1	8.7	23.5	30.0	5.0	20.1	25.7
57 PT	13.5	17.6	19.8	10.4	14.7	16.6	7.8	11.7	15.1	8.3	24.5	31.2	5.0	21.1	27.1
58 FR	13.5	17.6	19.8	10.4	14.7	16.6	7.8	11.7	15.1	8.3	24.5	31.2	5.0	21.1	27.1
59 TL	13.5	20.0	21.1	11.8	15.3	18.7	8.3	13.5	16.5	15.8	17.7	35.7	7.7	25.5	30.2
60 PO	16.0	20.9	23.4	12.3	15.7	19.6	8.7	13.7	16.0	16.8	28.3	37.7	7.9	26.4	31.0
61 PO'	17.4	22.8	25.1	13.5	15.8	18.1	9.1	13.7	17.1	11.6	30.5	30.2	8.0	23.5	33.5
62 AI	18.1	23.1	26.8	13.5	15.8	18.1	9.3	13.7	17.1	11.6	30.5	30.2	8.0	23.5	33.5
63 BM	18.1	23.1	26.8	13.5	15.8	18.1	9.3	13.7	17.1	11.6	30.5	30.2	8.0	23.5	33.5
64 FR	18.4	24.5	29.2	15.1	21.3	25.9	10.6	16.1	19.1	11.1	35.7	37.2	8.0	27.9	37.1
65 AC	20.9	25.5	27.2	15.1	21.3	25.9	11.1	16.1	19.1	11.1	35.7	37.2	8.0	27.9	37.1
66 TD	22.8	30.5	33.9	17.2	20.3	27.3	12.0	18.1	21.6	11.7	35.7	35.3	9.8	31.0	31.8
67 U	23.5	31.1	32.7	18.4	21.3	25.1	12.9	18.3	22.9	12.7	35.7	35.3	9.8	31.0	31.8
68 MP	25.9	34.8	39.0	19.1	27.0	30.5	13.7	20.4	37.5	9.2	35.0	33.2	10.9	34.6	37.3
69 AN	27.0	32.1	34.9	20.5	27.0	30.6	13.0	21.1	26.6	9.2	35.0	34.0	11.1	35.5	39.5
70 CH	27.5	37.6	42.7	21.1	30.2	34.3	10.2	16.4	26.7	10.1	28.1	37.3	11.1	37.1	48.3
71 CF	28.0	35.1	37.7	22.1	31.9	35.7	15.1	21.3	37.0	10.7	30.7	41.7	10.5	36.5	57.3

K₀ IS THE VALUE OF $\Delta f^*/(f_0 + \Delta f)$ CORRESPONDING TO THE FORWARD DIRECTION ($\theta = 0$). THE QUANTITIES K_{50'} AND K_{90'} DENOTE THE AVERAGE VALUES OF K CORRESPONDING TO THE RANGES $\theta = 0$ TO 50° AND $\theta = 0$ TO 90° RESPECTIVELY.

be taken to be constant. The fractional number of reciprocal lattice points within this elementary shell is

$$(4\pi H^2 dH)/(\int_0^{H_1} 4\pi H^2 dH) = (3H^2 dH)/H_1^3. \quad (1)$$

The value of \bar{k} for the range $H = 0$ to H_1 (i.e. $s = 0$ to s_1) can be obtained by taking a weighted average of k , the weight for the value of k in an elementary shell of radius H being the fractional number of reciprocal points in that shell. We thus have

$$\bar{k} = \frac{3}{H^{\frac{1}{3}}} \int_0^{H_1} k(H) H^2 dH \quad (2)$$

Since $H=2s$, (2) can also be written as

$$k = \frac{3}{s_1^3} \int_0^{s_1} k(s) s^2 ds \quad . \quad (3)$$

Equation (3) was used for obtaining the value of \bar{k} . The theoretical values $\Delta f'$ and $\Delta f''$ which are needed for the computation of \bar{k} are taken from Cromer & Liberman (1970) for the $K\alpha_1$ radiations and from Hazell (1967) for the $K\beta_1$ radiations. It has been found to be convenient to evaluate the atomic scattering factors for various values of s by an analytical method from the constants given by Cromer (1965). The values of the wavelengths for the $K\alpha_1$ and the $K\beta_1$ radiations necessary for evaluating s_1 occurring in (3) have been taken from Vol. III of *International Tables for X-ray Crystallography* (1962). The integration involved in (3) was carried out for each atom and wavelength by a numerical procedure on the IBM-1130 computer of this Centre. The values of k_0 , \bar{k}_{50° and \bar{k}_{90° for the $K\alpha_1$ radiations of Cr, Fe, Cu, Mo and Ag are given in Table 1 and those for the $K\beta_1$ of these target elements in Table 2.

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