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Relativistic Hartree-Fock X-ray and Electron Scattering Factors

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(Received 2 November 1967)

Kinematic X-ray and electron scattering factors, found with the use of relativistic Hartree-Fock atomic fields, are tabulated for 76 atoms and ions. Parametric fits to these are given in the range of $\sin \theta/\lambda$ from 0.0 to 2.0 Å⁻¹. A method is developed to obtain the electron structure factor for forward scattering for a crystal containing ionized atoms.

Introduction

A relativistic Hartree–Fock (R–HF) atomic wave function calculation has been programmed by Coulthard (1967). Results have been obtained by him and by the present authors for 76 atoms and ions. The calculation yields, among other data, the total charge densities $\varrho(r)$ and atomic potentials $\varphi(r)$. From these, kinematic scattering factors for X-rays and electrons, $f_X(s)$ and $f_{el}(s)$, have been found by using the equations

$$f_X(s) = 4\pi \int_0^\infty r^2 \varrho(r) \, \frac{\sin(4\pi sr)}{(4\pi sr)} \, dr \tag{1}$$

and

$$f_{el}(s) = \frac{8\pi^2 m_0 e}{h^2} \int_0^\infty r^2 \varphi(r) \, \frac{\sin(4\pi s r)}{(4\pi s r)} \, dr \,, \qquad (2)$$

where $s = \sin \theta / \lambda \text{ Å}^{-1}$.

Equation (2) was used only for neutral atoms. The case of ions will be dealt with separately. For asymmetric atoms, Harada & Kashiwase (1962) found $\underset{s\to 0}{\overset{\text{Lt}}{\overset{\text{s}}{\text{s}}}} f_{el}(s)$ depends on the direction in which the limit is taken. A single value is obtained in the present case, since the atom is considered as being spherically symmetrical.

A brief comparison, for mercury, between the R-HF scattering curves and those found from some other atomic models has been given previously (Doyle & Turner, 1967). Work by several authors (see Byron &

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Joachin, 1967*a*, *b*) has taken some account of correlations between electrons in the atom. However, since this deals only with a few light atoms, the present tabulation may prove useful. The inclusion of correlations might be expected to decrease $f_X(s)$ for medium *s*, and to increase $f_{el}(s)$ for small and medium *s*. Except for the lightest atoms, the most sophisticated tables previously available were those based on the nonrelativistic Hartree–Fock model by Freeman (1959) for lighter atoms, and on the Dirac–Slater model (relativ-



Fig. 1. $f_{Na}(s) + f_{C1}(s)$ for (a) neutral and (b) ionized atoms.

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Table 1. Kinematic X-ray scattering factors

s	HE	LI	LI+	BE	BE2+	В	С	N	٥	F	NE	NA	NA+
	ne 2.000 1.957 1.637 1.663 1.460 1.254 0.613 0.509 0.353 0.248 0.177 0.129 0.055 0.033 0.021 0.014 0.002 0.004 0.001 0.001 0.000 0.000	L1 3.000 2.708 2.215 1.904 1.742 1.626 1.393 1.270 1.149 1.033 0.650 0.512 0.404 0.320 0.404 0.320 0.404 0.320 0.404 0.320 0.404 0.004 0.004 0.002 0.001	2.000 1.984 1.936 1.861 1.762 1.648 1.523 1.394 1.266 1.141 1.024 0.815 0.643 0.507 0.400 0.317 0.400 0.317 0.400 0.317 0.400 0.021 0.044 0.021 0.001 0.002 0.001	4.000 3.707 3.065 2.463 2.060 1.828 1.692 1.400 1.520 1.443 1.362 1.362 1.95 1.030 0.876 0.740 0.622 0.439 0.311 0.223 0.163 0.120 0.060 0.012 0.005 0.003	2.000 1.992 1.966 1.925 1.870 1.803 1.726 1.641 1.458 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.364 1.365 1.79 1.007 0.853 0.425 0.301 0.216 0.1157 0.019 0.011 0.005 0.003	5 5.000 4.724 4.060 3.316 2.639 2.263 1.799 1.681 1.596 1.526 1.1576 1.526 1.147 1.020 0.900 0.524 0.304 0.233 0.126 0.072 0.012 0.006	6.000 5.749 5.107 4.311 3.560 2.949 2.171 1.948 1.794 1.685 1.537 1.426 1.322 1.219 1.114 0.736 0.588 0.468 0.373 0.468 0.373 0.025 0.013	N 7.000 6.180 5.385 4.563 3.219 2.747 2.393 2.132 1.942 1.942 1.551 1.455 1.353 1.265 0.921 0.769 0.636 0.525 0.324 0.088 0.023	8.000 7.798 7.245 6.472 5.623 4.089 3.489 3.029 2.338 1.377 1.221 1.070 0.926 0.792 0.674 0.443 0.292 0.134 0.037	9.000 8.815 8.302 7.560 6.709 5.054 4.353 3.270 2.874 1.956 1.588 1.482 1.324 1.186 1.055 0.928 0.810 0.564 0.389 0.270 0.055	NE 10.000 9.830 9.351 8.643 7.805 6.928 6.079 5.302 4.617 4.029 3.535 2.296 1.971 1.609 1.418 1.280 1.158 1.041 0.929 0.680 0.489 0.351 0.254 0.137 0.079	NA 11.000 10.568 9.760 9.027 8.335 7.618 6.156 5.471 4.848 4.293 2.754 2.305 1.997 1.784 1.367 1.247 1.137 1.032 0.791 0.591 0.438 0.325 0.107	10.000 9.883 9.546 9.026 8.374 6.8974 6.160 5.471 4.845 4.290 3.753 2.753 2.753 2.753 1.927 1.524 1.367 1.524 1.137 1.246 1.137 1.032 0.791 0.438 0.325 0.183 0.107
s	MG	MG2+	AL	SI	P	S	CL	CL-	AR	ĸ	K+	CA	CA2+
0.00 0.05 0.15 0.25 0.35 0.40 0.45 0.50 0.670 0.70 0.80 1.20 1.20 1.40 1.60 2.50 3.50 5.00 5.00 5.00 5.00	12.000 11.507 10.472 9.502 8.078 7.446 6.194 5.034 4.059 2.317 2.729 2.317 2.022 1.660 1.459 1.326 1.459 1.326 1.459 1.326 0.691 0.527 0.401 0.234 0.141	10.000 9.914 9.262 9.265 8.751 8.156 6.210 5.5925 5.025 5.025 4.046 3.288 2.724 2.023 1.662 1.218 1.419 0.890 0.689 0.526 0.400 0.233 0.141	13.000 12.439 11.230 10.059 9.158 8.465 7.316 6.766 6.222 4.713 3.221 2.330 1.841 1.571 1.408 1.292 1.195 0.979 0.783 0.615 0.478 0.290 0.179	14.000 13.434 12.134 10.769 9.673 8.859 8.231 7.698 7.202 6.240 5.312 4.470 3.164 2.702 2.076 1.717 1.505 1.367 1.264 1.656 0.867 0.556 0.349 0.222	$15.000 \\ 14.458 \\ 13.138 \\ 11.629 \\ 10.327 \\ 9.335 \\ 8.600 \\ 8.029 \\ 7.547 \\ 7.103 \\ 6.674 \\ 5.829 \\ 7.547 \\ 7.103 \\ 1.626 \\ 1.453 \\ 1.333 \\ 1.122 \\ 0.942 \\ 0.777 \\ 0.632 \\ 0.411 \\ 0.268 \\ 0.531 \\$	16.000 15.484 14.177 12.583 11.109 9.039 8.376 7.856 7.856 7.856 7.417 6.254 5.505 4.138 3.570 2.133 1.779 2.133 1.557 1.411 1.182 1.009 0.849 0.316	17.000 16.511 15.234 13.597 11.991 10.633 9.576 8.181 7.706 6.595 5.245 4.607 4.6023 3.070 1.967 1.686 1.502 1.2405 1.502 1.2405 1.502 1.2405 1.502 0.773 0.536 0.367	18.000 17.330 15.685 13.747 11.987 10.580 9.524 8.1629 7.305 6.600 5.248 4.024 3.070 5.2405 1.968 1.502 1.2405 1.502 1.2405 1.502 0.536 0.367	$18.000 \\ 17.536 \\ 16.298 \\ 14.647 \\ 12.949 \\ 11.441 \\ 10.216 \\ 9.272 \\ 8.558 \\ 8.011 \\ 7.575 \\ 6.875 \\ 5.639 \\ 5.036 \\ 4.460 \\ 2.713 \\ 2.192 \\ 1.844 \\ 1.614 \\ 1.614 \\ 1.614 \\ 1.614 \\ 1.614 \\ 1.614 \\ 0.836 \\ 0.597 \\ 0.419 \\ 0.419 \\ 0.419 \\ 0.836 \\ 0.597 \\ 0.419 \\ 0.610 \\ 0.597 \\ 0.419 \\ 0.610 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597 \\ 0.419 \\ 0.597$	19.000 18.204 16.733 13.728 12.268 10.977 9.908 9.061 8.403 7.125 5.961 5.406 4.859 3.045 2.450 2.033 1.748 1.367 1.174 1.028 0.657 0.472	$18.000 \\ 17.649 \\ 16.677 \\ 13.297 \\ 13.760 \\ 9.056 \\ 8.399 \\ 7.886 \\ 7.125 \\ 5.962 \\ 5.406 \\ 4.859 \\ 3.045 \\ 2.449 \\ 3.045 \\ 2.033 \\ 1.749 \\ 1.367 \\ 1.174 \\ 1.028 \\ 0.657 \\ 0.471 \\$	20.000 19.091 17.331 15.723 14.304 12.961 11.705 10.590 9.650 8.885 8.275 7.392 6.228 5.717 5.209 4.233 3.391 2.733 2.250 1.908 1.444 1.225 1.078 0.524	18.000 17.721 16.935 15.774 14.412 13.017 10.575 9.629 8.262 7.389 6.764 6.731 5.209 4.232 3.390 0.2.732 2.250 1.909 1.444 1.225 1.078 0.9715 0.524
S	sc	TI	v	¥2+	CR	MN	MN2+	FE	FE2+	FE3+	co	C02+	NI
0.00 0.05 0.10 0.25 0.30 0.35 0.40 0.50 0.50 0.50 0.50 0.50 0.50 1.00 1.20 1.40 1.40 1.60 1.800 2.500 2.500 3.500 6.000	21.000 20.131 16.356 16.645 13.732 12.423 11.244 10.226 9.377 7.682 6.996 6.460 5.501 4.570 3.722 3.023 2.485 2.090 1.533 1.279 1.125 0.998 0.770 0.577	22.000 21.171 19.410 17.635 16.044 14.572 13.198 11.999 10.852 9.920 9.148 8.007 7.240 9.148 8.007 7.240 5.752 4.872 4.038 3.316 2.734 2.290 1.637 1.338 1.171 1.044 0.821 0.627	23.000 22.208 20.474 18.661 17.003 15.465 14.026 12.705 11.530 9.660 8.373 7.5060 6.892 6.406 5.972 5.139 4.333 3.604 2.992 2.506 1.756 1.2750 1.530 1.5407 1.5305 1.5407 1.5305 1.5407 1.5407 1.5305 1.5407 1.5305 1.5407 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5305 1.5305 1.5407 1.5305 1.5407 1.5305 1.5407 1.5407 1.5305 1.5407 1.5407 1.5305 1.5407 1.5407 1.5305 1.5407 1.5305 1.5407 1.5505 1.5407 1.5505 1.5407 1.5505 1.5407 1.5505 1.5407 1.5607	21.000 20.702 19.861 18.618 17.146 15.602 14.107 12.736 11.5300 10.500 9.641 8.359 7.501 6.892 6.407 5.973 5.137 4.330 3.600 2.989 2.505 1.756 1.404 1.217 1.087 0.868 0.676	24.000 23.329 21.789 20.022 18.260 16.561 14.965 13.513 12.227 11.118 6.165 7.791 7.118 6.406 6.172 5.372 4.597 3.874 3.244 4.3.244 2.727 1.888 1.479 1.266 1.129 0.914 0.724	$\begin{array}{c} 25.000\\ 24.274\\ 12.611\\ 20.764\\ 19.012\\ 17.364\\ 15.806\\ 14.353\\ 13.031\\ 11.858\\ 6.353\\ 13.031\\ 11.858\\ 6.353\\ 8.137\\ 7.368\\ 6.359\\ 5.586\\ 4.849\\ 4.144\\ 3.506\\ 4.849\\ 4.144\\ 3.506\\ 1.319\\ 1.563\\ 1.319\\ 1.956\\ 0.769\\ \end{array}$	23.000 22.707 21.875 20.629 19.126 17.517 15.920 14.417 13.055 11.857 10.827 9.128 7.365 6.808 6.360 5.585 4.846 4.140 3.502 2.960 2.037 1.563 1.319 1.171 0.956 0.769	26.000 25.304 23.678 21.829 20.046 18.354 15.233 13.845 11.502 9.512 7.645 5.070 4.388 3.195 2.197 1.658 1.377 1.213 0.995 0.813	$\begin{array}{c} 24.000\\ 23.711\\ 22.889\\ 21.649\\ 20.140\\ 18.508\\ 16.871\\ 13.881\\ 12.606\\ 11.494\\ 9.737\\ 8.501\\ 7.640\\ 7.023\\ 6.546\\ 5.775\\ 5.068\\ 4.384\\ 3.749\\ 3.192\\ 2.196\\ 1.658\\ 1.377\\ 1.213\\ 0.995\\ 0.812\end{array}$	23.000 22.763 22.078 21.023 19.705 18.238 16.727 15.254 13.877 12.630 11.531 9.772 8.523 7.651 7.026 6.548 5.074 4.392 3.757 3.199 2.199 16.659 1.377 1.213 0.995 0.812	27.000 26.331 24.744 22.900 21.093 19.364 17.709 16.145 14.695 13.379 12.209 10.309 8.930 7.955 7.259 6.738 5.950 5.270 4.613 3.989 3.424 2.366 1.763 1.441 1.258 3.033 0.853	25.000 24.716 23.904 22.673 21.164 19.516 17.845 16.236 14.743 13.396 12.207 10.293 8.917 7.948 7.257 6.739 5.951 5.268 4.609 3.985 3.421 2.365 1.763 1.441 1.258 1.033 0.853	28.000 27.356 25.807 23.973 22.150 20.390 18.696 12.956 10.909 9.392 8.301 7.519 6.944 6.118 5.576 11.059 8.301 7.519 6.944 6.118 5.4819 4.211 3.647 2.543 1.376 1.512 1.306 1.059 0.892

Table 1 (cont.)

s	NI2+	CU	CU+	ZN	ZN2+	GA	GE	AS	SE	BR	BR-	KR	RB
0.00 0.05 0.10 0.120 0.25 0.355 0.4550 0.500 0.500 0.500 1.000 1.400 1.400 1.400 1.400 1.600 2.000 3.500 5.000 6.000	26.000 25.721 23.702 22.195 20.536 18.839 17.187 15.637 14.224 12.962 10.895 9.378 8.292 7.516 6.944 6.119 5.450 4.816 4.207 3.643 2.5541 1.877 1.512 1.336 1.069 0.892	29.000 28.448 27.084 25.370 21.687 19.869 18.133 16.514 13.707 11.5034 13.707 9.861 8.663 7.799 7.166 6.285 5.617 5.005 5.617 5.005 5.413 3.855 2.721 2.001 1.590 1.358 1.105 0.929	28.000 27.663 26.711 25.294 21.770 19.939 18.180 16.541 15.047 13.710 11.502 9.855 8.659 7.797 7.165 5.617 5.603 4.411 3.853 2.719 2.000 1.358 1.105 0.929	30.000 29.401 27.927 26.124 24.283 20.720 19.027 17.421 15.926 14.559 10.442 9.108 8.132 7.417 6.453 5.775 5.180 4.610 4.063 2.908 2.135 1.677 1.414 1.140 0.964	28.000 27.732 26.958 25.766 24.275 22.606 20.869 19.149 17.504 14.580 12.227 8.126 7.414 6.455 5.775 5.178 4.606 4.059 2.095 2.134 1.677 1.414 1.140 0.964	31.000 30.308 28.675 26.783 24.935 23.174 21.481 19.847 18.278 16.794 15.410 12.976 15.410 12.976 4.510 7.702 6.633 5.926 5.342 4.792 4.260 3.097 2.277 1.772 1.477 1.176 0.998	32.000 31.276 29.534 27.504 25.567 23.791 22.136 20.560 19.047 17.598 16.227 13.770 11.7598 16.227 13.770 11.745 10.151 1.1745 10.151 8.937 8.028 6.830 6.076 5.493 4.961 4.447 3.2428 1.876 1.545 1.213 1.030	33.000 32.274 30.473 28.307 26.235 24.386 22.724 19.725 18.326 16.989 14.535 12.442 10.741 8.396 7.050 6.231 5.636 5.117 4.621 3.475 2.584 1.251 1.261	34.000 33.280 31.449 29.175 26.962 25.001 23.288 18.977 17.682 15.269 13.145 11.362 9.928 8.809 7.299 6.395 5.775 5.262 4.782 3.658 2.745 2.108 1.703 1.292 1.092	35.000 34.291 32.450 25.658 23.857 22.288 20.874 19.558 18.307 15.958 13.837 12.001 10.480 9.262 7.580 6.574 5.913 5.398 4.932 3.839 4.932 3.839 1.337 1.123	36.000 35.077 32.827 30.175 27.706 25.595 23.812 22.2264 20.867 19.550 18.313 15.964 13.840 12.002 10.479 9.261 7.580 6.573 5.913 5.913 5.938 4.932 3.836 2.909 2.235 1.793 1.337 1.123	36.000 35.304 33.467 31.055 28.590 26.364 24.453 22.820 21.388 20.087 18.870 16.594 14.504 12.645 11.057 9.752 7.898 6.773 6.056 5.528 5.671 4.007 3.074 2.369 1.384 1.154	37.000 35.946 33.907 31.681 29.368 27.146 25.158 23.432 21.934 20.605 19.391 17.167 15.126 13.272 11.645 26.996 6.210 5.656 5.200 4.168 3.239 2.507 1.939 1.436 1.186
s	RB+	SR	SR2+	MO	AG	CD	IN	SN	SN2+	SN4+	SB	I	1-
0.00 0.05 0.10 0.15 0.25 0.35 0.45 0.50 0.45 0.50 0.45 0.50 0.40 1.20 1.20 1.20 1.20 1.20 0.3 5.00 3.50 3.50 3.50 3.50 5.00 5.00	36.000 35.435 33.891 31.740 29.393 27.147 25.150 23.424 21.929 20.603 19.391 17.169 15.128 13.273 11.645 10.270 8.251 6.997 6.209 5.656 5.201 4.168 3.239 2.507 1.993 1.436 1.186	38.000 36.802 34.458 32.171 29.988 27.863 25.875 24.090 22.522 21.141 19.902 17.696 15.702 13.872 12.230 10.806 8.640 7.249 6.376 5.785 5.323 4.320 3.401 2.649 3.401 2.649 1.219	36.000 35.524 34.198 32.281 30.089 27.892 25.861 24.064 22.500 21.128 19.898 17.700 15.707 13.875 12.231 10.805 8.638 7.249 6.375 5.785 5.785 5.785 5.324 4.320 3.401 2.648 2.103 1.493 1.219	42.000 41.003 38.656 35.907 33.195 30.665 28.382 26.368 24.620 23.109 21.796 17.732 16.036 14.448 12.968 10.430 8.542 7.251 6.397 5.813 4.827 3.988 3.217 2.581 1.766 1.373	47.000 46.139 43.964 41.157 36.154 35.192 32.416 29.910 27.707 25.805 24.181 18.069 16.651 15.316 12.813 10.623 8.869 7.569 6.651 15.351 4.566 3.862 3.207 2.206 1.635	48.000 47.085 44.797 41.923 38.930 36.007 33.251 30.725 28.468 26.492 24.784 22.063 20.027 18.405 17.000 15.698 13.253 11.060 9.249 7.867 6.871 5.461 4.665 3.977 3.330 2.304 1.698	49.000 47.980 45.534 42.603 36.774 34.059 31.538 29.247 27.209 25.425 22.408 18.736 17.329 16.053 13.670 11.492 9.639 8.184 7.110 5.577 4.761 4.087 3.449 2.406 1.764	50.000 48.934 46.361 43.309 40.302 37.462 37.462 36.794 22.303 30.011 27.938 26.096 23.081 120.815 19.073 17.646 16.384 14.062 11.913 10.034 8.516 7.367 5.702 4.853 4.192 3.565 2.509 1.835	48.000 47.373 45.650 43.206 40.431 37.604 34.878 30.008 27.920 26.075 23.067 19.075 23.067 19.074 17.649 16.386 14.063 11.913 10.033 8.515 7.367 5.702 4.853 4.191 3.565 2.509 1.834	46.000 45.590 44.404 42.572 37.718 35.082 32.517 30.127 27.972 26.074 23.019 20.767 19.052 17.646 16.395 14.074 11.917 10.033 8.513 7.366 5.702 4.853 4.190 3.563 2.508 1.834	51.000 49.915 47.250 44.056 38.100 35.465 28.663 26.784 23.646 21.253 19.424 17.958 16.696 14.429 12.321 10.431 8.861 7.642 5.836 4.945 4.2945 4.2945 2.615 1.909	53.000 51.911 49.142 45.702 42.340 39.333 36.675 30.030 28.141 24.851 22.228 20.193 18.599 17.293 15.090 13.082 11.214 9.576 8.239 6.142 5.132 4.478 3.891 2.828 2.067	54.000 52.646 49.413 45.698 42.265 39.276 32.082 30.040 28.149 24.855 22.227 15.091 13.082 11.214 9.577 8.239 6.142 5.132 4.478 3.891 2.828 2.067
	s	XE	cs	CS+	ва	EU	AU	HG	PB	BI	RN	U	
	0.00 0.05 0.10 0.20 0.25 0.35 0.40 0.40 0.40 0.45 0.50 0.70 0.80 0.70 0.80 0.90 1.20 1.40 1.60 1.20 1.40 1.60 1.20 2.50 3.50 4.00 5.00 6.00	54.000 52.917 50.125 46.588 43.088 39.9671 37.251 34.850 32.671 30.656 28.785 25.470 22.758 20.618 18.943 17.591 13.432 1.5922 9.940 8.5566 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.5661 3.991 2.561 3.991 2.5661 3.991 2.561 3.991 2.561 3.991 2.561 3.991 2.561 3.991 2.561 3.991 3.935 2.150 3.550 3.550 3.935 3.550 3.550 3.935 3.550 3.550 3.550 3.550 3.550 3.550 3.550 3.550 3.550 3.591 3.550 3.591 3.550 3.591 3.550 3.591 3.550 3.591 3.550 3.591 3.591 3.591 3.591 3.592 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.591 3.520 3.591 3.550 3.591 3.550 3.	55.000 53.527 50.603 47.291 43.888 40.713 37.904 35.440 33.241 31.236 29.382 26.072 23.303 21.072 19.310 17.900 17.900 13.759 10.303 8.881 6.502 5.332 4.087 3.041 2.237	54.000 53.084 50.635 47.345 40.703 37.893 35.434 33.240 31.238 29.385 23.303 21.071 19.309 17.900 11.95676 13.7606 10.302 8.882 5.332 4.0851 4.087 3.041 2.237	56.000 54.345 51.122 47.839 44.456 38.598 36.063 33.818 29.948 26.652 23.851 21.547 19.701 18.224 19.701 18.2553 14.0675 10.661 9.213 6.704 5.4400 4.178 3.146 2.325	63.000 61.552 55.228 51.847 48.444 45.176 42.160 39.433 36.980 34.761 27.576 27.576 27.576 27.576 17.789 15.841 14.2459 20.565 17.763 15.841 12.763 11.345 8.348 6.433 5.378 4.750 3.812 2.965	79.000 77.936 75.135 71.380 67.296 63.241 59.395 55.835 55.835 52.581 49.622 46.929 42.207 38.153 34.581 31.387 28.530 23.789 20.287 17.821 16.081 14.770 12.168 9.826 7.878 6.489 5.010 4.244	80.000 78.899 72.198 68.038 64.029 60.177 56.600 53.318 50.326 47.601 42.829 35.176 31.980 29.112 24.303 20.692 18.116 16.298 14.949 8.081 6.644 5.090 4.310	82.000 80.750 77.607 73.645 69.530 61.712 58.138 54.820 51.766 48.969 44.969 44.969 30.252 25.350 21.546 18.754 16.764 15.317 12.724 10.482 8.495 6.973 5.260 4.441	83.000 81.700 78.438 74.365 70.203 66.204 62.4255 55.563 52.495 49.669 44.700 40.501 36.879 33.680 30.805 21.992 19.097 17.017 15.510 12.896 10.690 8.704 7.145 5.351 4.505	86.000 84.649 76.737 72.258 68.109 64.332 60.862 57.631 54.604 51.767 46.659 42.281 38.533 35.277 32.389 27.426 23.379 20.215 17.859 16.143 13.386 11.282 9.329 7.686 5.650 4.702	92.000 86.130 81.595 77.080 72.712 68.607 64.838 61.409 55.410 50.268 45.784 41.869 38.454 35.458 30.391 26.192 22.699 19.886 17.713 14.341 12.294 10.495 8.823 6.378 7.378	

Table 2. Kinematic electron scattering factors*

* These values must be multiplied by $m/m_0 = (1 - v^2/c^2)^{-1/2}$ for electrons of velocity v.

	2	3	4	5	6	7	8	9	10	11	12	13	14
s	ΗE	LI	36	3	с	N	0	F	NE	NA	MG	AL	S I
0.00 0.05 0.10 0.25 0.30 0.40 0.45 0.50 0.60 0.70 0.80 1.20 1.40 1.60 2.00 2.50 2.50 0.90 1.20 2.50 0.90 1.20 2.50 0.90 1.20 0.90 1.50 0.90 1.50 0.90 0.75 0.90 0.75 0.90 0.75 0.90 0.75 0.90 0.75 0.90 0.75 0.90 0.90 0.90 0.90 0.90 0.90 0.90 0.9	0.418 0.410 0.359 0.250 0.250 0.217 0.139 0.164 0.143 0.110 0.068 0.068 0.068 0.065 0.046 0.032 0.024 0.015 0.015 0.015 0.0015 0.005 0.005 0.003 0.005	3.286 2.800 1.879 1.166 0.753 0.254 0.259 0.188 0.145 0.219 0.188 0.145 0.046 0.028 0.003 0.002	3.052 2.807 2.237 1.635 1.151 0.635 0.614 0.371 0.302 0.253 0.136 0.145 0.117 0.059 0.059 0.235 0.028 0.228 0.015 0.011 0.008 0.004 0.003	$\begin{array}{c} 2.794\\ 2.638\\ 2.250\\ 1.791\\ 1.377\\ 1.048\\ 0.803\\ 0.625\\ 0.497\\ 0.402\\ 0.333\\ 0.239\\ 0.144\\ 0.118\\ 0.078\\ 0.072\\ 0.055\\ 0.043\\ 0.035\\ 0.028\\ 0.019\\ 0.013\\ 0.010\\ 0.007\\ 0.005\\ 0.003\end{array}$	2.509 2.405 2.138 1.795 1.463 0.932 0.748 0.606 0.497 3.141 3.297 0.175 0.141 3.141 3.141 3.141 5.051 0.051 0.034 0.022 0.015 0.004 0.009 0.005 0.009 0.005	$\begin{array}{c} 2.211\\ 2.144\\ 1363\\ 1.718\\ 1.458\\ 1.216\\ 1.006\\ 0.831\\ 0.689\\ 0.575\\ 0.484\\ 0.353\\ 0.208\\ 0.167\\ 0.137\\ 0.098\\ 0.167\\ 0.137\\ 0.098\\ 0.047\\ 0.039\\ 0.026\\ 0.018\\ 0.010\\ 0.007\\ 0.005\end{array}$	1.983 1.937 1.808 1.625 1.422 1.040 0.747 0.635 0.542 0.403 0.241 0.193 0.159 0.113 0.085 0.066 0.053 0.044 0.029 0.020 0.012 0.008 0.005	1.801 1.767 1.671 1.532 1.371 1.206 1.049 0.908 0.784 0.445 0.445 0.445 0.445 0.445 0.445 0.272 0.219 0.128 0.074 0.025 0.074 0.049 0.032 0.049 0.032 0.023 0.013 0.009 0.006	$\begin{array}{c} 1.652\\ 1.626\\ 1.552\\ 1.443\\ 1.313\\ 1.176\\ 1.043\\ 0.805\\ 0.706\\ 0.619\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.479\\ 0.019\\ 0.003\\ 0.066\\ 0.025\\ 0.015\\ 0.009\\ 0.007\end{array}$	4.778 4.138 2.967 2.099 1.594 1.295 1.095 0.926 0.827 0.727 0.642 0.505 0.403 0.325 0.266 0.221 0.158 0.117 0.092 0.073 0.059 0.028 0.021 0.016 0.007	5.207 4.717 3.656 2.657 1.953 1.502 1.211 1.013 0.868 0.757 0.567 0.528 0.425 0.239 0.172 0.129 0.100 0.065 0.043 0.030 0.022 0.017 0.011 0.008	5.889 5.371 4.237 3.128 2.299 1.363 1.110 0.932 0.801 0.700 0.551 0.366 0.304 0.255 0.189 0.109 0.087 0.024 0.025 0.024 0.029 0.024 0.029 0	5.828 5.421 4.467 3.437 2.589 1.969 1.9534 1.017 0.861 0.743 0.578 0.383 0.320 0.198 0.198 0.117 0.093 0.076 0.035 0.026 0.020 0.013 0.009
	15	16	17	18	19	20	21	22	23	24	25	26	27
S	P	s	CL	AR	к	CA	sc	τı	v	CR	MN	FE	co
0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.40 0.40 0.40 0.40 0.40 0.40 0.40	5.488 5.192 4.457 3.586 2.796 2.169 1.702 1.362 1.115 0.933 0.797 0.610 0.487 0.401 0.335 0.284 0.210 0.160 0.125 0.100 0.082 0.037 0.028 0.021 0.014	5.161 4.938 4.362 3.927 1.851 1.490 1.218 1.014 0.648 0.648 0.648 0.648 0.648 0.649 0.350 0.419 0.350 0.221 0.169 0.133 0.107 0.087 0.057 0.030 0.023 0.010	4.857 4.685 4.227 3.620 2.997 2.438 1.974 1.606 1.319 1.098 0.428 0.692 0.541 0.366 0.311 0.232 0.178 0.178 0.141 0.113 0.0693 0.062 0.031 0.024 0.031 0.024 0.031	4.580 4.444 4.074 3.566 3.022 2.512 2.070 1.705 1.412 1.181 0.998 0.740 0.574 0.462 0.383 0.324 0.242 0.187 0.148 0.119 0.045 0.033 0.026 0.033 0.026 0.017 0.012	8.984 7.619 5.426 3.997 3.154 2.578 2.134 1.776 1.487 1.252 1.064 0.402 0.402 0.402 0.402 0.402 0.402 0.194 0.156 0.127 0.047 0.047 0.025 0.012	9.913 6.388 4.550 3.408 2.695 2.206 1.838 1.548 1.314 1.123 0.838 0.647 0.515 0.422 0.162 0.132 0.137 0.071 0.037 0.028 0.013	9.307 8.318 6.328 4.633 3.509 2.783 2.281 1.906 1.374 1.179 0.885 0.684 0.544 0.544 0.544 0.544 0.544 0.544 0.544 0.521 0.169 0.137 0.169 0.137 0.075 0.039 0.030 0.019 0.014	8.776 7.937 6.199 4.643 3.564 2.844 2.341 1.964 1.428 1.428 1.428 1.428 1.428 0.930 0.721 0.573 0.467 0.285 0.143 0.175 0.143 0.078 0.117 0.078 0.041 0.031 0.020 0.014	8.305 7.581 6.045 4.616 3.588 2.386 2.011 1.716 1.476 1.476 1.277 0.973 0.602 0.490 0.490 0.297 0.490 0.148 0.122 0.081 0.043 0.021 0.015	6.969 6.427 5.291 3.434 2.403 2.403 1.761 1.523 1.014 0.514 0.514 0.514 0.514 0.154 0.127 0.085 0.042 0.085 0.060 0.022 0.015	$\begin{array}{c} 7.506\\ 6.949\\ 5.719\\ 3.583\\ 2.924\\ 2.445\\ 2.080\\ 1.553\\ 1.356\\ 1.047\\ 0.659\\ 0.538\\ 0.659\\ 0.538\\ 0.446\\ 0.323\\ 0.246\\ 0.159\\ 0.159\\ 0.132\\ 0.088\\ 0.062\\ 0.046\\ 0.023\\ 0.016\\ \end{array}$	$\begin{array}{c} \textbf{7.165} \\ \textbf{6.669} \\ \textbf{5.558} \\ \textbf{4.436} \\ \textbf{3.562} \\ \textbf{2.928} \\ \textbf{2.461} \\ \textbf{2.104} \\ \textbf{1.818} \\ \textbf{1.584} \\ \textbf{1.584} \\ \textbf{1.584} \\ \textbf{1.584} \\ \textbf{0.686} \\ \textbf{0.561} \\ \textbf{0.686} \\ \textbf{0.561} \\ \textbf{0.466} \\ \textbf{0.255} \\ \textbf{0.202} \\ \textbf{0.165} \\ \textbf{0.202} \\ \textbf{0.136} \\ \textbf{0.637} \\ \textbf{0.637} \\ \textbf{0.637} \\ \textbf{0.6217} \end{array}$	6.854 6.410 5.401 3.534 2.924 2.471 1.841 1.610 1.416 1.110 0.883 0.712 0.583 0.350 0.265 0.209 0.170 0.141 0.094 0.0047 0.039 0.039 0.025 0.017
	28	29	30	31	32	33	34	35	36	37	38	42	47
S	NI	CU	ZN	GA	GE	AS	SE	BR	KR	RB	SR	MU	AG
0.00 0.05 0.10 0.20 0.20 0.23 0.45 0.445 0.45 0.445 0.460 0.70 0.80 0.90 1.20 1.400 1.800 2.500 3.550 4.000 5.0000 5.0000 5.0000 5.0000 5.00000 5.000000000000000000000000000000000000	6.569 4.283 3.500 2.914 2.474 2.133 1.858 1.631 1.440 0.909 0.737 0.605 0.217 0.146 0.097 0.069 0.052 0.040 0.026 0.018	5.600 5.287 4.595 3.267 2.320 2.428 2.123 1.868 1.651 1.464 1.163 0.761 0.626 0.523 0.761 0.626 0.378 0.285 0.285 0.2224 0.150 0.150 0.151 0.072 0.054 0.027 0.019	6.065 5.735 4.962 4.123 3.421 2.850 2.468 2.144 1.882 1.663 1.181 0.955 0.781 0.646 0.541 0.391 0.296 0.155 0.104 0.074 0.055 0.028 0.019	7.108 6.629 5.564 4.486 3.629 2.997 1.903 1.679 1.492 1.197 0.973 0.800 0.665 0.405 0.306 0.240 0.194 0.160 0.107 0.057 0.024 0.029	7.378 6.935 5.902 4.783 3.849 3.143 2.623 2.235 1.938 1.702 1.212 0.989 0.817 0.681 0.317 0.681 0.248 0.200 0.165 0.110 0.059 0.024 0.021	7.320 6.953 6.048 4.992 4.048 3.299 2.733 2.308 1.986 1.734 1.533 1.228 1.304 0.697 0.431 0.327 0.256 0.206 0.170 0.113 0.081 0.081 0.081 0.081	7.205 6.895 6.105 5.132 4.211 3.446 2.849 2.393 2.045 1.776 1.562 1.245 1.019 0.847 0.711 0.603 0.444 0.337 0.264 0.212 0.175 0.116 0.083 0.062 0.048 0.0022	7.060 6.795 6.104 5.217 4.339 3.578 2.963 2.484 2.113 1.825 1.598 1.266 1.034 0.725 0.616 0.456 0.4456 0.4456 0.4456 0.272 0.219 0.180 0.119 0.085 0.064 0.050 0.022 0.023	6.670 6.064 5.260 4.434 3.690 2.575 2.186 1.881 1.640 1.290 1.050 0.873 0.467 0.280 0.467 0.280 0.225 0.185 0.185 0.183 0.088 0.066 0.033 0.023	11. 773 10.073 7.402 5.658 4.566 3.149 2.651 2.254 1.938 1.686 1.319 1.068 1.319 1.068 0.887 0.749 0.640 0.478 0.365 0.233 0.188 0.126 0.090 0.052 0.034 0.024	13.109 11.476 8.478 8.200 4.794 3.882 2.315 1.993 1.733 1.733 1.350 1.089 0.902 0.762 0.651 0.488 0.375 0.297 0.2397 0.194 0.129 0.0649 0.054 0.035 0.024	10.260 9.548 8.004 6.481 5.269 4.341 3.622 3.054 2.600 2.233 1.934 1.490 1.185 0.525 0.408 0.525 0.408 0.325 0.263 0.216 0.101 0.076 0.039 0.027	8.244 7.267 6.215 5.293 3.878 3.339 2.886 2.505 2.185 1.688 1.335 1.688 1.335 1.688 0.454 0.454 0.357 0.2568 0.454 0.357 0.2241 0.159 0.113 0.084 0.066 0.043 0.030

Table 2 (cont.)

	48	49	50	51	53	54	55	56	63	79	80	82	83
S,	CD	IN	SN	53	I	×E	CS	BA	EU	AU	НG	PB	BI
0.00 0.05 0.15 0.25 0.35 0.40 0.50 0.60 0.70 0.80 1.20 0.90 1.20 0.80 1.200 2.500 3.000 3.000 5.000 6.000	9.232 8.764 7.666 6.464 5.427 4.592 3.375 2.922 2.542 2.223 1.724 1.366 1.107 0.916 0.451 0.362 0.297 0.246 0.163 0.115 0.086 0.067 0.044 0.031	10.434 9.768 8.207 5.601 4.682 2.973 3.412 2.955 2.576 2.257 1.758 1.397 0.587 0.789 0.587 0.250 0.168 0.308 0.308 0.250 0.118 0.088 0.245 0.231	$10.859 \\ 10.209 \\ 8.709 \\ 7.118 \\ 5.803 \\ 4.801 \\ 4.044 \\ 3.453 \\ 2.990 \\ 2.608 \\ 2.288 \\ 1.790 \\ 2.608 \\ 2.288 \\ 1.426 \\ 1.157 \\ 0.956 \\ 0.805 \\ 0.597 \\ 0.465 \\ 0.307 \\ 0.255 \\ 0.170 \\ 0.255 \\ 0.170 \\ 0.069 \\ 0.045 \\ 0.032 \\ 0.045 \\ 0.032 \\ 0.032 \\ 0.032 \\ 0.045 \\ 0.005 \\ 0.045 \\ 0.$	10.974 10.387 8.976 7.386 6.010 4.940 4.131 3.514 3.030 2.640 2.318 1.819 1.453 1.181 0.821 0.603 0.472 0.379 0.173 0.122 0.091 0.071 0.046 0.033	10.905 10.434 9.235 7.764 6.379 5.234 4.341 3.658 3.130 2.715 2.380 1.871 1.503 1.227 1.016 0.855 0.630 0.487 0.321 0.268 0.179 0.127 0.095 0.073 0.048 0.034	$10.794 \\ 10.371 \\ 9.274 \\ 7.884 \\ 6.529 \\ 5.374 \\ 4.454 \\ 3.742 \\ 3.191 \\ 2.414 \\ 1.897 \\ 1.2759 \\ 2.414 \\ 1.897 \\ 1.248 \\ 1.036 \\ 0.871 \\ 0.642 \\ 0.495 \\ 0.397 \\ 0.325 \\ 0.272 \\ 0.183 \\ 0.130 \\ 0.097 \\ 0.034 \\ 0$	$16.508 \\ 14.106 \\ 10.525 \\ 8.201 \\ 6.649 \\ 5.471 \\ 4.547 \\ 3.822 \\ 3.255 \\ 2.809 \\ 2.453 \\ 1.923 \\ 1.548 \\ 1.269 \\ 1.055 \\ 0.888 \\ 0.654 \\ 0.502 \\ 0.405 \\ 0.332 \\ 0.132 \\ 0.132 \\ 0.098 \\ 0.050 \\ 0.035 \\ 0.035 \\ 0.035 \\ 0.035 \\ 0.035 \\ 0.035 \\ 0.000 \\ 0.035 \\ 0.000 \\ 0$	18.267 15.854 11.675 8.682 6.829 5.570 4.628 3.318 2.861 1.951 1.570 1.288 1.073 0.904 0.666 0.511 0.337 0.277 0.189 0.134 0.0078 0.036	$15.563 \\ 13.867 \\ 10.722 \\ 8.267 \\ 6.673 \\ 5.574 \\ 4.740 \\ 4.072 \\ 3.525 \\ 3.075 \\ 2.703 \\ 2.136 \\ 1.429 \\ 1.016 \\ 0.752 \\ 0.457 \\ 0.372 \\ 0.307 \\ 0.209 \\ 0.150 \\ 0.150 \\ 0.087 \\ 0.067 \\ 0.067 \\ 0.067 \\ 0.067 \\ 0.040 \\ 0.067 \\ 0.067 \\ 0.040 \\ 0.067 \\ 0.067 \\ 0.060 \\ 0.067 \\ 0.067 \\ 0.060 \\ 0.067 \\ 0$	$10.573 \\ 10.195 \\ 9.251 \\ 8.106 \\ 7.003 \\ 5.214 \\ 4.526 \\ 3.952 \\ 3.472 \\ 3.070 \\ 2.446 \\ 1.995 \\ 1.661 \\ 1.407 \\ 1.208 \\ 0.717 \\ 0.572 \\ 0.465 \\ 0.384 \\ 0.256 \\ 0.184 \\ 0.139 \\ 0.108 \\ 0.071 \\ 0.050 \\ 0.050 \\ 0.050 \\ 0.050 \\ 0.050 \\ 0.051 \\ 0.050 \\ 0.050 \\ 0.051 \\ 0.050 \\ 0.$	$10.964 \\ 10.555 \\ 9.533 \\ 8.299 \\ 7.128 \\ 6.116 \\ 5.272 \\ 4.572 \\ 3.991 \\ 3.507 \\ 2.471 \\ 2.015 \\ 1.676 \\ 1.419 \\ 1.218 \\ 0.926 \\ 0.724 \\ 0.579 \\ 0.471 \\ 0.389 \\ 0.259 \\ 0.471 \\ 0.389 \\ 0.186 \\ 0.141 \\ 0.110 \\ 0.072 \\ 0.050 \\ 0.$	$12.597 \\ 11.979 \\ 10.516 \\ 8.888 \\ 7.461 \\ 6.310 \\ 5.395 \\ 4.066 \\ 3.573 \\ 2.522 \\ 2.052 \\ 1.708 \\ 1.444 \\ 1.239 \\ 0.942 \\ 0.738 \\ 0.591 \\ 0.482 \\ 0.399 \\ 0.265 \\ 0.190 \\ 0.144 \\ 0.112 \\ 0.073 \\ 0.052 \\ 0.52 \\ 0.52 \\ 0.52 \\ 0.52 \\ 0.52 \\ 0.516 $	13.096 12.456 10.921 9.186 4.432 5.472 4.714 4.104 4.104 3.606 3.191 2.546 2.076 2.576 0.548 0.488 0.488 0.408 0.268 0.488 0.405
	86	92			з	4	11	12	17	19	20	23	25
s	RN	U			LI+	BE2+	NA+	MG2+	CL-	к+	CA2+	¥2÷	MN2+
0.00 0.05 0.15 0.25 0.35 0.40 0.50 0.60 0.50 0.60 0.70	13.492 12.949 11.565 9.854 8.223 6.852 4.912 4.244 3.711 3.277 2.616 2.135 1.475 1.499 1.283 0.974 0.765 0.503 0.418 0.278 0.150 0.117 0.054	19.119 17.436 14.059 8.928 7.387 6.221 5.307 4.576 3.985 3.503 2.775 1.5875 1.5875 1.5875 1.585 1.024 0.803 0.649 0.534 0.443 0.212 0.159 0.124 0.082 0.058			0.157 9.730 2.546 1.212 0.740 0.518 0.393 0.259 0.189 0.145 0.093 0.145 0.046 0.046 0.046 0.027 0.064 0.046 0.027 0.064 0.003 0.002 0.011 0.008 0.002 0.004 0.003 0.002	0.082 19.229 4.867 2.207 1.274 0.841 0.605 0.461 0.300 0.252 0.188 0.118 0.097 0.035 0.025 0.035 0.025 0.005 0.005 0.0006 0.0004 0.003	$\begin{array}{c} 1.130\\ 10.692\\ 3.480\\ 2.100\\ 1.571\\ 1.284\\ 1.092\\ 0.946\\ 0.827\\ 0.642\\ 0.506\\ 0.403\\ 0.325\\ 0.266\\ 0.221\\ 0.157\\ 0.118\\ 0.091\\ 0.015\\ 0.039\\ 0.028\\ 0.021\\ 0.016\\ 0.010\\ 0.007\\ \end{array}$	0.831 19.972 5.595 2.909 1.944 1.472 1.103 0.866 0.757 0.668 0.529 0.529 0.172 0.286 0.239 0.172 0.129 0.100 0.080 0.065 0.043 0.030 0.043 0.030 0.022 0.017 0.011 0.008	6.770 -3.162 3.147 3.461 3.000 2.458 1.988 1.613 1.322 1.099 0.928 0.691 0.439 0.364 0.311 0.232 0.178 0.141 0.113 0.060 0.024 0.024 0.024 0.011	3.436 12.939 5.559 3.939 3.135 2.175 2.135 1.778 1.488 1.253 1.064 0.789 0.488 0.402 0.195 0.125 0.125 0.027 0.012	2.711 21.817 7.336 4.495 3.343 2.674 2.204 1.551 1.316 1.124 0.838 0.647 0.515 0.422 0.203 0.161 0.108 0.071 0.050 0.037 0.028 0.013	2.904 22.005 7.514 4.661 3.833 2.365 2.005 1.716 1.279 0.973 0.973 0.490 0.408 0.490 0.408 0.228 0.181 0.123 0.081 0.021 0.015	2.846 21.953 7.479 4.650 3.514 2.865 2.415 2.068 1.357 1.553 1.357 1.049 0.538 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.446 0.459 0.132 0.088 0.046 0.033 0.016
	26	26	27	28	29	30	35	37	38	50	50	53	55
S	FE2+	FE3+	C02+	NI2+	C U+	ZN2+	BR-	R8+	SR2+	SN2+	SN4+	I-	CS+
0.05 0.15 0.20 0.20 0.230 0.350 0.45 0.45 0.60 0.700 1.200 1.200 1.200 1.200 1.200 1.460 1.800 2.500 3.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 2.500 3.500 4.000 4.000 2.500 3.500 4.000 4.000 2.500 3.500 4.000 4.000 2.500 3.500 4.000 5.000	2.802 21.913 7.447 4.629 3.506 2.428 2.088 1.813 1.583 1.583 1.583 1.389 1.081 0.687 0.561 0.466 0.236 0.256 0.336 0.202 0.164 0.091 0.065 0.048 0.037 0.024 0.024 0.017	2.296 3).996 4.388 5.294 3.767 2.466 2.099 1.813 1.580 1.385 1.079 0.854 0.561 0.561 0.561 0.561 0.256 0.336 0.256 0.336 0.256 0.364 0.365 0.091 0.065 0.044 0.037 0.227	$\begin{array}{c} 2.754\\ 21.867\\ 7.409\\ 4.603\\ 3.492\\ 2.866\\ 2.103\\ 1.833\\ 1.608\\ 1.416\\ 1.111\\ 0.883\\ 0.713\\ 0.583\\ 0.485\\ 0.350\\ 0.265\\ 0.209\\ 0.170\\ 0.141\\ 0.094\\ 0.067\\ 0.050\\ 0.025\\ 0.017\\ \end{array}$	2.703 21.819 7.368 4.572 3.473 2.856 2.436 2.436 2.436 2.436 1.628 1.628 1.628 1.628 1.628 1.628 1.628 0.504 0.364 0.275 0.504 0.364 0.217 0.176 0.146 0.097 0.069 0.052 0.040 0.052	3.280 12.803 5.479 3.942 3.234 2.769 2.410 2.114 1.864 1.649 1.464 1.163 0.935 0.761 0.627 0.523 0.378 0.286 0.224 0.182 0.150 0.101 0.072 0.054 0.027 0.019	2.599 21.719 7.282 4.504 3.426 2.831 2.428 2.120 1.869 1.658 1.476 0.956 0.541 0.295 0.646 0.541 0.292 0.185 0.104 0.075 0.043 0.025 0.028 0.019	9.357 -0.738 5.202 5.132 4.365 3.602 2.975 2.975 2.975 1.598 1.266 1.034 0.860 0.725 0.616 0.456 0.456 0.457 0.272 0.219 0.180 0.119 0.085 0.064 0.050 0.0052 0.023	5.545 14.987 7.442 5.595 3.773 3.151 2.652 2.254 1.938 1.686 0.318 1.068 0.318 0.749 0.4478 0.366 0.288 0.290 0.470 0.090 0.052 0.052 0.034 0.024	$\begin{array}{c} 4.642\\ 23.704\\ 9.101\\ 6.084\\ 4.734\\ 3.871\\ 3.228\\ 2.723\\ 2.319\\ 1.994\\ 1.733\\ 1.089\\ 0.902\\ 0.902\\ 0.902\\ 0.902\\ 0.902\\ 0.902\\ 0.238\\ 0.196\\ 0.238\\ 0.129\\ 0.092\\ 0.054\\ 0.129\\ 0.054\\ 0.054\\ 0.024\end{array}$	$\begin{array}{c} 6.144 \\ 25.152 \\ 10.411 \\ 7.227 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.725 \\ 5.75 \\ \mathbf$	3.971 42.227 13.395 7.902 5.818 4.703 3.967 3.416 2.973 2.604 2.2911 1.794 1.428 0.956 0.597 0.465 0.374 0.306 0.255 0.170 0.120 0.090 0.045 0.032	13.835 3.399 8.586 7.767 6.423 5.255 4.348 3.658 3.658 3.129 2.714 2.379 1.871 1.503 1.227 1.017 0.855 0.487 0.391 0.321 0.321 0.321 0.127 0.075 0.073 0.048	9.035 18.344 10.448 8.143 3.6.643 5.475 4.549 3.823 1.548 1.269 1.055 0.888 0.654 0.504 0.300 0.276 0.300 0.276 0.132 0.076 0.132 0.076

istic Hartree with a Slater statistical approximation to exchange) for all atoms (Cromer & Waber, 1965).

The atoms chosen in the accompanying tables represent a compromise between the desire to complete the periodic table, and the computing time available. Some light atoms such as helium for which better approximations have been calculated (see *International Tables for X-ray Crystallography*, Vol.III) were included, for completeness, and because they take little time. Coulthard's R-HF program is probably capable of treating most atoms, though F^- failed to converge, and difficulty may be met in dealing with some transition metals and rare earths.

Kinematic scattering from ionized atoms

 $f_{el}(s)$ has generally been obtained from the Mott formula for $s \neq 0$. For s=0, the values $\pm \infty$ are found for an ion. It is desirable to find finite values at s=0that can be used in a neutral unit cell containing ions.

Z		^a 1	^b 1	^a 2	^b 2	^a 3	^b 3	^a 4	^b 4	c	Е
2	на	0.8734	9.1037	0.5309	3.3563	0.3112	22.9276	0.1780	0.9821	0.0054	0.0084
3	LI	1.1282	3.9546	0.7503	.05?4	0.6175	85.3905	0.4653	168.2610	0.0377	0.0512
з	LI+	0.6958	4.6237	0.7888	1.9557	0.3414	0.6316	0.1563	10.0953	0.0157	0.0017
4	ΒE	1.5919	43.6427	1.1278	1.8623	0.5391	103.4830	0.7029	0.5420	0.0385	0.0224
4	BE 2+	6.2603	0.0027	0.8849	0.8313	0.7993	2.2758	0.1647	5.1146	-6.1092	0.0102
5	8	2.0545	23.2185	1.3376	1.0210	1.0979	60.3498	0.7063	0.1403	-0.1932	0.0152
6	С	2.3100	20.8439	1.0200	10.2075	1.5886	0.5687	0.8650	51.6512	0.2156	0.0244
7	N	12.2126	0.0057	3.1322	9.8933	2.0125	28.9975	1.1663	0.5826	-11.5293	0.0357
8	e	•3.0485	13.2771	2.2963	5.7011	1.5463	0.3239	0.8670	32.9089	0.2508	0.0041
.9	F	.3.5392	10.2825	2.6412	4.2944	1.5170	0.2015	1.0243	20.14/0	0.2116	0.0054
10	NE NE	3.9353	8.4042	2011/2	304:02	1 2676	0.2300	1 1120	120 4541	0.5515	0.0740
11	NA	4.1020	2 66 71	2 0242	200422	1 3009	0.2001	1.0032	14.0590	0-4040	0.0027
12	NC	5.4204	2.8575	2.1735	79.261	1.2269	0.3208	2.3073	7,1977	0.8584	0.0379
12	₩G2+	3.4988	2.1676	3.8378	4.7542	1.3284	0.1850	0.8497	10.1411	0.4853	0.0013
13	AL	6.4202	3.0387	1.9002	0.7426	1.5936	31.5472	1.9646	35.0886	1.1151	0.0444
14	SĪ	6.2915	2.4386	3.0353	32.3337	1.9891	0.6785	1.5410	81.6937	1.1407	0.0167
15	Ρ	6.4345	1.9067	4.1791	27.1570	1.7800	0.5260	1.4908	68.1645	1.1149	0.0075
16	S	6.9053	1.4679	5.2034	22.2151	1.4379	0.2536	1.5863	56.1720	0.8669	0.0132
17	CL	11.4604	0.0104	7.1964	1.1662	6.2556	18.5194	1.6455	47.7784	-9.5574	0.0196
17	CL-	18.2915	0.0066	7.2084	1.1717	6.5337	19.5424	2.3386	60.4486	-16.3776	0.0204
18	AR	7.4845	0.9072	.6.7723	14.8407	0.6539	43.8983	1.6442	33.3929	1.4445	0.0438
19	ĸ	8.2186	12.7949	7.4398	0.7748	1.0519	213.1869	0.8659	41.6841	1.4228	0.0284
19	K+	1.9518	12.0331	7 2072	0.1514	1 5000	-0.0020	1 0211	3109140	-4.9970	0.0374
20	CA24	8.0200	10.44/1	7 0519	0.6099	1.0899	30 2116	1.0211	25.0005	-14.9751	0.0291
20	50	9,1890	9.0213	7.3679	0.5729	1.6409	136,1083	1.4660	51.3531	1.3329	0.0356
22	11	9.7595	7.8508	7.3558	0.5000	1.6991	35.6338	1.9021	116.1046	1.2807	0.0306
23	Î,	10.2971	6.8657	7.3511	0.4385	2.0703	26.8938	2.0571	102.4778	1.2199	0.0248
23	v2+	10.1060	6.8818	7.3541	0.4409	2.2884	20.3004	0.0223	115.1221	1.2298	0.0255
24	CR	10.6406	6.1038	7.3537	0.3920	3.3240	20.2626	1.4922	98.7399	1.1832	0.0189
25	MN	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896	0.0169
25	₩N2+	10.8061	5.2796	7.3620	0.3435	3.5268	14.3430	0.2184	41.3235	1.0874	0.0130
26	FE	11.7695	4.7611	7.3573	0.3072	3.5222	15.3535	2.3045	76.8805	1.0369	0.0162
26	FE3+	11.1764	4.6147	7.3863	0.3005	3.3948	11.6729	0.0724	38.5566	1 0007	0.0095
20	rt2+	12 29/2	4.0038	7 3400	0 2794	4.1340	12.00040	2.2488	71.1692	1.0118	0.0170
27	C02+	11.2296	4-1731	7.3883	0.2726	4.7393	10.2443	0.7108	25.6466	0.9324	0.0052
28	NI.	12.8376	3.8785	7.2920	0.2565	4.4438	12.1763	2.3800	66.3421	1.0341	0.0184
28	NI2+	11.4166	3.6766	7.4005	0.2449	5.3442	8.8730	0.9773	22.1626	0.8614	0.0031
29	CU	13.3380	3.5828	7.1576	0.2470	5.6158	11.3966	1.6735	64.8126	1.1910	0.0206
29	CL+	11.9475	3.3669	7.3573	0.2274	6.2455	8.6625	1.5578	25.8487	0.8900	0.0038
30	ZN	14.0743	3.2655	7.0319	0.2333	5.1652	10.3163	2.4100	58 . 7097	1.3041	0.0210
30	ZN2+	11.9719	2.9946	7.3862	0.2031	6.4668	7.0826	1.3940	18.0995	0.7807	0.0016
31	C A	15.2354	3.0669	6.7006	0.2412	4.3591	10.7805	2.9623	61.4135	1.1189	0.0302
32	GE	16.0816	2.8509	6.3/4/	0.2647	3.4313	12.9479	4.2779	240 1022	2.5310	0.0268
34	АЗ 5 F	17.0006	2-4098	5.8196	0-2726	3,9731	15.2272	4.3543	43.8163	2.8409	0.0208
25	PR	17.1789	2.1723	5.7358	16.5796	5.6377	0.2609	3,9851	41.4328	2.9557	0.0139
35	BR-	17.1718	2.2059	6.3338	19.3345	5.5754	0.2871	3.7272	58.1535	3.1776	0.0200
		17 0555	1 0201	4 72.04	14 5422	E E403	0 2261	3 5375	30 3072	2 9250	0 0074
36	KK	17.3355	1 7000	0.4435	17 3151	5.5495	0.2769	1.5207	144.0330	2.4873	0.0286
31	K D D D A	17 5016	1.7130	7.6598	14.7957	5-8981	0.1603	2.7817	31,2087	2.0782	0.0017
38	50	17.5663	1.5564	9.8184	14.0988	5.4220	0.1664	2.6694	132.3758	2.5064	0.0180
38	SR 2+	18-0874	1.4907	8.1373	12.6963	2.5654	24.5651	-34-1929	-0.0138	41.4025	0.0071
42	MO	3.7025	0.2772	17.2356	1.0958	12.8876	11.0040	3.7429	61.6584	4.3875	0.0384
47	AG	19.2808	0.6446	16.6885	7.4726	4.8045	24.6605	1.0463	99.8156	5.1790	0.0174
48	CD	19.2214	0.5946	17.6444	6.9089	4.4610	24.7008	1.6029	87.4825	5.0694	0.0206
49	IN	19.1624	0.5476	18.5596	6.3776	4.2948	25.8499	2.0396	92.8029	4.9391	0.0224
50	SN	19.1889	5.8303	19.1005	0.5031	4.4585	26.8909	2.4663	83.9571	4.7821	0.0228
50	SN2+	19.1094	0.5036	19.0548	5.8378	4.5648	23.3752	0.4870	62.2061	4.7861	0.0233
50	SN4+	18,9333	5.7640	19.7131	0.4655	3.4182	14.0049	0.0193	-0.7583	3.9182	0.0111
51	58	19.6418	5.3034	19.0455	0.4007	7 6139	27 7660	2.0021	1202022	4.0712	0.0223
23	1.	20+14/2	4.3570	19.99747	0.3815	7-8069	29.5259	2.8868	84.9304	4.0714	0.0207
55	XF	20.2933	3.9282	19.0298	0.3440	8.9767	26.4659	1.9900	64.2658	3.7118	0.0201
55	ĉŝ	20.3892	3.5690	19.1062	0.3107	10.6620	24.3879	1.4953	213.9036	3.3352	0.0206
55	čš+	20.3524	3.5520	19.1278	0.3086	10.2821	23.7128	0.9615	59.4565	3.2791	0.0196
56	8 A	20.3361	3.2160	19.2970	0.2756	10.8880	20.2073	2.6959	167.2022	2.7731	0.0186
63	EU	24.6274	2.3879	19.0886	0.1942	13.7603	13.7546	2.9227	123-1737	2.5745	0.0200
79	AU	16.8819	0.4611	18.5913	8.6216	25.5582	2.4826	5,8600	36.3956	12.0658	0.0233
80	HG	20.6809	0.5450	19.0417	8.4484	21.6575	1.5729	5.9676	38.3246	12.6089	0.0247
82	PB	31.0617	0.6902	13.0637	2.3576	18+4420	8.6180	5.9696	4/02579	13 5700	0.0296
83	81	35.5689	0.440	12.9510	2.9238	1000077	8 1931	7.4433	40.0093	13.6905	0.0147
92		36.0228	0.5293	23.4128	3.3253	14.9491	16.0927	4.1880	100.6130	13.3966	0.0143

Table 3. Parameters for the fit of $f_X(s)$

Defining

$$\varphi^{1}(r) = \varphi(r) - \frac{e\Delta Z}{4\pi\varepsilon_{0}r}$$

where ΔZ is the ionic charge, (2) can be written as

$$f_{el}(s) = \frac{8\pi^2 m_0 e}{h^2} \int_o^\infty r^2 \varphi^1(r) \ \frac{\sin(4\pi sr)}{(4\pi sr)} dr + \frac{m_0 e^2 \Delta Z}{8\pi h^2 \epsilon_0 s^2} .$$
(3)

This simply separates the coulomb field due to the excess or deficiency of charge on the nucleus from the remaining atomic field. The Fourier transform of a coulomb field, used to find the second term of (3), was evaluated originally by Bethe (1930). Values of $f_{el}(s)$ for $s \neq 0$ listed in Table 2 for ions were found by the use of (3), which is equivalent to using the Mott formula.

For s=0, the amplitude scattered from a crystal depends on the zero-order Fourier coefficient of potential

$$V_0 = \frac{1}{\Omega} \int V(\mathbf{r}) d\mathbf{r}$$

where Ω is the unit cell volume, and $V(\mathbf{r})$ the crystal field potential. V_0 is independent of ion positions in the unit cell. If all coulomb fields due to the excess and deficiency of charge on the nuclei in the unit cell are superimposed with their centres coincident, then they give a net contribution of zero to $V(\mathbf{r})$. Thus for any ion positions in a neutral unit cell, the structure factor depends only on the first term in (3), and it is these values which are given in Table 2 for s=0.

The (200), (400), ... structure factors for the fundamental cell of NaCl depend on $f_{Na}(s) + f_{Cl}(s)$. Fig. 1 shows this sum for neutral atoms and for singly ionized atoms. The value at s=0 is lower for the ionic case, showing the more effective screening of the nuclear fields by the ionized atoms.

Calculations

Values of $\rho(r)$ and $\varphi(r)$ are computed by Coulthard's program at up to 180 points, exponentially weighted towards the nucleus. Repeated use of an equal-interval formula based on 7 points (the 'six-strip rule') was employed for the numerical integration of (1) and (2) (see, for example, Abramowitz & Stegun (1965), p.886). Although the third (and probably also the second)

Table 4(a). Parameters for the fit of $f_{el}(s)$. Neutral atoms

Z		^a 1	^b 1	a,	^b 2	^a 3	^b 3	^a 4	^b 4	Е
2	HS	0.0906	18.1834	0.1814	6.2109	0.1095	1.8026	0.0362	0.2844	0.0220
3	LI	1.6108	107.6384	1.2460	20.4795	0.3257	4.5331	0.09.16	0.4951	0.0849
4	βE	1.2498	60.8042	1.3335	18-5914	0.3603	3-6534	0.1055	0.4:57	0.0629
5	P	0.9446	46.4438	1.3120	14.1778	0.4188	3.2228	0.1159	0.3767	0.0569
6	ċ	0.7307	35.9951	1,1951	11.2966	0.4567	2.8139	0.1247	0 3456	0.0500
7	Ň	0.5717	28.8465	1.0425	9.0542	0.4647	2.4213	0.1211	0.2167	0.0399
8	n i	0.4548	23.7803	0.9173	7.6220	0.4719	2 1440	0 1204	0.3050	0.0370
ğ	Ē	0.3686	20.2390	0.8109	6.6093	0.4751	1 0310	0 1/50	0.2703	0.0526
10	NE	0-3025	17.6390	0.7202	5.8604	0 4751	1 7422	0 1 5 3 4	0.2/95	0.0205
11	N A	2.2406	108.0030	1 2274	26 E047	0.0070	2 2014	0.1554	0.2000	0.0215
12	NG	2.2692	73.6704	1 9025	20 1740	0.9070	3. 3914	0.2005	0.4548	0.1208
13	A 1	2.2756	72 2220	2 4 2 90	10 7720	0 0 5 7 9	3.0700	0.2592	0.4046	0.0883
14	51	2.1203	57 7740	2 5 2 2 2	3701127	0.03/0	3.0799	0.3106	0.4076	0.0896
15	Ĵ,	1.8882	44 8754	2.4405	12 5202	0.0044	2.00/90	0.3210	0.3860	0.0757
16	ċ	1.4591	36.6500	2 3043	11 4001	0.7000	2.0424	0.3204	0.3508	0.0617
17	cĭ.	1.4574	30.0352	2 2024	1104001	0 7074	2.0000	0.3208	0.3403	0.0515
10		1 2724	34 4033	2 1006	7.7190	0.7074	2.0000	0.3217	0.3228	0.0437
10	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	3 0507	127 0749	201094	3.6150	0.7927	2.2186	0.3225	C.3071	0.0370
20	C Å	4.4696	99.5729	2 0709	22.04017	1 0404	4.3519	0.4017	0 4 3 4 0	0.1379
21	ŝr	3.9459	98.0507	2 0140	20 6041	1 0 2 5 4	2 0557	0.4010	0.4105	0.1094
22	TT	3.5653	81.0821	2.0101	10 04 04	1 9030	3 5004	0.4002	0.3966	0.1045
23	ŷ	3.2449	75.3789	2.6978	17.7262	1.8507	3 3433	0 4025	0 37/3	0.1019
24	C.R.	2.3066	78-4051	2 3330	15,7851	1,9224	3 1544	0.4004	0 3 4 3 4	0.1102
25	MN	2.7467	67.7862	2.4556	15.6743	1.7923	2 0000	0 4001	0.3540	0.1102
26	FF	2.5440	64-4244	2.3434	14.5906	1.7599	2 9530	0 5047	0.3503	0.0958
27	ĊĒ	2.3668	61-4306	2.2361	14 1700	1 7343	2.0000	0.5062	0.3502	0.0943
28	NT	2.2104	58-7267	2.1342	13 5520	1 4 9 0 .	2 6004	0.5330	0.33442	0.0928
29	ci.	1.5792	62.9403	1.8197	12-4527	1.6576	2.5047	0 5323	0 33 31	0.1006
30	7 N	1.9418	54.1621	1.9501	12.5177	1.6192	2 6166	0 5/3/	0.33351	0.1004
31	G A	2.3205	65.6019	2.4955	15.4577	1.6970	2 5804	0.5002	0.3510	0.1035
32	GE	2.4467	55.8930	2.7015	14.3930	1.6157	2.4461	0.6009	0.3415	0.0970
33	۵S	2.3989	45.7179	2.7898	12. 8166	1.5799	2 2700	0.5034	0.3377	0.0370
34	SE	2.2980	38-8296	2.8541	11.5359	1.4555	2.1463	0 5995	0.3143	0.0507
35	BR	2.1659	33,8987	2.9037	10.4004	1.3051	2 0413	0 5092	0 3070	0.0597
36	KR	2.0338	29.9992	2.9271	9.5977	1-3425	1.9520	0.5888	0 2096	0.0453
37	RB	4.7760	140.7821	3.8588	18,9910	2.2339	3.7010	0.8683	0.2700	0.1550
38	SR	5.8478	104.9721	4.0026	19-3666	2.3420	3.7368	0.8795	0 4142	0.1313
42	MC	3.1199	72.4642	3,9061	14-6424	2.3615	3,2370	0.8504	0.3662	0 10 9
47	AG	2.0355	61.4970	3.2716	11.8237	2.5105	2.8456	0.8372	0.3271	0.0049
48	CD	2.5737	55.6752	3.2586	11.8376	2-5468	2.7842	0.8379	0.3217	0.0956
49	IN	3.1528	66.6492	3.5565	14.4494	2.8180	2.9758	0.8842	0.3345	0.1025
50	SN	3.4495	59.1042	3.7349	14.1787	2.7779	2.8548	0.8786	0.3270	0.0900
51	SB	3.5644	50.4869	3.8437	13.3156	2.6866	2.6909	0.8638	0-3161	0.0764
53	1	3.4728	39.4411	4.0602	11.8161	2.5215	2.4148	0.8348	0.2976	0.0581
54	ΧE	3.3656	35.5094	4.1468	11.1170	2.4430	2.2940	0.8293	0.2892	0.0513
55	C S	6.0620	155.8336	5.9861	19.6951	3.3033	3.3354	1.0958	0.3793	0.1567
56	84	7.8212	117.6575	6.0040	18.7782	3.2803	3.2634	1.1030	0.3760	0.1375
63	εu	6.2667	100.2983	4.8440	16.0662	3.2023	2.9803	1.2009	0.3674	0.1375
79	۸U	2.3880	42.8656	4.2259	9.7430	2.6886	2.2641	1.2551	0.3067	0.0774
80	⊦G	2.6817	42.8217	4.2414	9.8557	2.7549	2.2951	1.2708	C.3067	0.0754
82	₽B	3,5099	52.9141	4.5523	11.8840	3.1539	2.5713	1.3591	0-3205	0.0907
83	ыI	3.8412	0.2608	4.6794	11.9988	3.1924	2.5598	1.3625	0.3177	0.0849
86	RN	4.0779	28.4058	4.9778	11.0204	3.0955	2.3549	1.3259	0.2991	0.0617
<u>92</u>	U	6.7668	85.9510	6.7287	15.6415	4.0135	2.9364	1.5607	C.3348	0.1187

Table 4(b). Parameters for the fit of $f_{el}(s)$. Ionized atoms

Z		Δz	^a 1	^ъ 1	^a 2	^b 2	^a 3	^b 3	^a 4	^b 4	Е
3	LI+	1	0.0538	1.0860	0.0208	7.6853	0.0587	3.1378	0.0237	0.1923	0.0082
4	8E2+	2	-0.0002	0.2171	0.0169	3.3691	0.0407	1.1282	0.0243	0.2008	0.0194
11	NA+	1	0.1677	11.2946	0.4740	4.2735	0.3590	1.4135	0.1289	0.2262	0.0092
12	MC2+	2	0.0989	8.1847	0.3315	3.3711	0.2886	1.1900	0.1118	0.1984	0.0045
17	CL-	-1	1.9290	50.1174	3.2667	13.4759	1.1666	3.0567	0.3972	0.3713	0.0729
19	K+	1	0.8880	18.3273	1.6382	6.7637	0.6271	1.8497	0.2816	0.2713	0.0220
20	CA2+	2	0.6443	13.8112	1.2902	5.5116	0.5242	1.6178	0.2523	0.2453	0.0135
23	V2+	2	0.4754	19.2254	1.3279	5.9361	0.7998	1.8605	0.2996	0.2538	0.0241
25	MN2+	2	0.4523	17.3232	1.2228	5.4583	0.8599	1.7444	0.3102	0.2422	0.0203
26	FE 2+	2	0.4328	16.4991	1.1715	5.2529	0.8819	1.6870	0.3157	0.2373	0.0187
26	FE3+	3	0.3133	12,3214	0.9929	4.3988	0.7149	1.5040	0,2771	0.2174	0.0106
27	C02+	2	0.4149	15.6581	1.1218	5.0435	0.8959	1.6265	0.3208	0.2323	0.0169
28	NI2+	2	0.3932	14.9689	1.0741	4.8695	0.9086	1.5730	0.3266	0.2283	0.0156
29	CU+	1	0.5401	20.5410	1.2368	5.9307	1.1176	1.7355	0.3843	0,2501	0.0276
30	ZN2+	2	0.3509	13.7756	0.9852	4.5632	0.9235	1.4749	0.3387	0.2212	0.0135
35	8R-	-1	2.8044	52.9153	4.1294	13.8053	1.7053	2.5144	0.7016	0.3511	0.0846
37	RB+	1	1.5652	21.4061	2.3080	7.6576	1.1424	1.6782	0.5270	0.2693	0.0285
38	SR 2+	2	1.2452	16.6652	1.9124	6.4532	1.0007	1.4964	0.4833	0.2483	0.0190
50	SN2+	2	1.4363	25.5762	2.2527	6.9676	1.7685	2.0370	0.6836	0.2641	0.0363
50	SN4+	4	0.6327	10.3654	1.8013	4.0965	1.0063	1.3935	0.5307	0.2129	0.0078
53	I –	-1	4.2495	59.6448	5.6512	15.5905	2.9603	2.7837	0.9489	0.3300	0.0873
55	CS+	1	2.7761	26.0552	3.3558	9.0139	2.1398	2.0273	0.7588	0.2654	0.0352

decimal places have no physical significance, the f(s) values are tabulated to three places as an aid to interpolation. Tables 1 and 2 list $f_X(s)$ and $f_{el}(s)$ respectively, for values of s up to 6.0 Å⁻¹. Values of $f_{el}(0)$ for ions are as described in the previous section.

Analytical approximations to f(s), of the form

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

where the a_i , b_i and c are parameters determined by curve fitting procedures, were introduced by Vand, Eiland & Pepinsky (1957) for X-ray scattering factors. Tables of $f_X(s)$ parameters for n=2 were published by Forsyth & Wells (1959), while Cromer & Waber (1965) fitted the Dirac-Slater $f_X(s)$ curves with the use of 9 parameters (n=4). Smith & Burge (1962) used six parameters (n=3, c=0) in fitting electron scattering factors.

A non-linear least-squares curve fitting computer program due to Marquardt* (1963) has been used to determine 9-parameter approximations to $f_X(s)$ and 8-parameter approximations (c=0) to $f_{el}(s)$. These are listed in Table 3 and Table 4(*a*) respectively. 201 values of the functions, evaluated in the range s=0.00 to 2.00were used. For $f_{el}(s)$, for ions, an additional term $0.023934\Delta Z/s^2$ was added to (4) for non-zero values of *s*. This is the contribution to $f_{el}(s)$ from the excess nuclear charge. The remaining eight parameters fit the Fourier transform of the non-coulombic atomic field, including s=0. Table 4(*b*) lists the eight parameters and the ionic charge for ionized electron scattering factors.

Since $f_{el}(s)$ asymptotes to a Lorentzian, a parametric fit using four Lorentzians was attempted. However, for s from 0.00 to 2.00, the fit was significantly inferior,

so that the Gaussian parameters of (4) were retained.

For each atom, the root mean square value E of the deviation δ_i between theoretical and fitted *f*-values is expressed as a percentage of f(0), *i.e.*

$$E = \frac{100}{f(0)} \left[\frac{\sum_{i=1}^{201} \delta_i^2}{201} \right]^{\frac{1}{2}}.$$

These are listed in the last columns of Tables 3 and 4. The difference between actual and predicted values is rarely greater than 0.02, and is usually about 0.005.

The authors are indebted to Mr M.A. Coulthard for permission to use his R-HF program, and to Mr D.J.H.Cockayne for helpful discussions on ionized atoms. Their thanks are also due to Dr F. Hirst of the University's Computation Department for permission to use the computer for extended periods, and to Messrs I.E. Pollard and P. M. Warburton for their help with computer operation.

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^{*} This program is available through *SHARE* [number 3094(PA)].