

Current Status of Electron Scattering Factor Calculations

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There are presented some new values of the atomic scattering amplitudes for electrons calculated from Hartree-Fock wave functions by means of the Born approximation.

The atomic scattering factor for electrons is a complex quantity, and some calculations of the magnitudes and phases of the atomic scattering factor were carried out about eight years ago^(1,2) and again very recently⁽³⁾. Such complex scattering factors are essential for the successful interpretation of electron diffraction patterns from molecules which contain both heavy and light atoms, and so their calculation, though arduous, is important. On the other hand, real atomic scattering amplitudes for electrons, calculated readily with the use of the Born approximation, find extensive application to the interpretation of electron diffraction patterns from solids and gases in those cases where the disparity in the phases of the scattering factors of the separate atoms can be neglected. Here we shall limit ourselves to a discussion of Born approximation atomic scattering amplitudes and provide a tabulation of new, more reliable values.

The atomic scattering amplitude for electrons $f(s)$, within the framework of the Born approximation, is related to the X-ray form factor $f_x(s)$ by

$$f(s) = (2me^2/\hbar^2)s^{-2}(Z - f_x(s))$$

where $s = \lambda^{-1}4\pi \sin \theta$, and 2θ is the scattering angle. A knowledge of atomic wave functions or potentials is necessary in order to evaluate $f_x(s)$ and $f(s)$.

Several tabulations of atomic scattering amplitudes for electrons have appeared in the last decade⁽⁴⁻⁷⁾, each additional tabulation either supplementing or replacing the previous one. The amplitudes in these tabulations were generally derived from the Thomas-Fermi-Dirac statistical atom for $Z > 20$, and by interpolation on available Hartree-Fock wave functions for $Z \leq 20$. Over the last few

years, largely owing to the efforts of A. J. Freeman and R. E. Watson, Hartree-Fock wave functions have become available for all atoms from H to Kr and for Ag. Such wave functions are generally more reliable than the statistical atom, and so scattering amplitudes based on them may also be more reliable. In the table below we have given some new values of atomic scattering amplitudes for electrons, based on these new Hartree-Fock wave functions.

A comparison of these calculations with previous ones provides some indications of the problems involved in attempting to arrive at a reliable set of atomic scattering amplitudes for electrons for spherically symmetric, neutral atoms. The amplitudes are very sensitive, particularly at low scattering angle, to the wave functions used, to exchange effects, to relativistic effects, and particularly to bonding or ionization. Yet the present tabulations of atomic scattering amplitudes, based on Hartree-Fock wave functions out to Kr, and generally on the Thomas-Fermi-Dirac statistical atom beyond that, are reliable to 10% or better from $\lambda^{-1} \sin \theta \geq 0.3$. The error increases at lower scattering angles and may be as large as 50-100% at $\lambda^{-1} \sin \theta$ of 0-0.1 \AA^{-1} .

References

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Table of f Values (in Å)

		$\lambda^{-1} \sin \theta$											
	Z	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.50	0.60	0.70
He	2	(0.445)	0.431	0.403	0.368	0.328	0.288	0.250	0.216	0.188	0.142	0.109	0.086
Ne	10	(1.66)	1.59	1.53	1.43	1.30	1.17	1.04	0.92	0.80	0.62	0.48	0.38
Al	13	(6.1)	5.36	4.24	3.13	2.30	1.73	1.36	1.11	0.93	0.70	0.55	0.45
Si	14	(6.0)	5.26	4.40	3.41	2.59	1.97	1.54	1.23	1.02	0.74	0.58	0.47
P	15	(5.4)	5.07	4.38	3.55	2.79	2.17	1.70	1.36	1.12	0.80	0.61	0.49
S	16	(5.2)	4.88	4.36	3.63	2.93	2.33	1.85	1.49	1.22	0.86	0.65	0.51
Cl	17	(5.0)	4.69	4.24	3.62	3.00	2.44	1.98	1.61	1.32	0.93	0.69	0.54
K	19	(9.0)	(7.0)	5.43	(4.10)	3.15	(2.60)	2.14	(1.90)	1.49	1.07	0.79	0.61
Sc	21	(9.7)	8.35	6.30	4.63	3.50	2.75	2.29	1.92	1.62	1.18	0.89	(0.69)
Ti	22	(8.9)	7.95	6.20	4.63	3.55	2.84	2.34	(1.97)	1.67	1.23	0.93	0.72
V	23	(8.4)	7.60	6.06	4.60	3.57	2.88	2.39	(2.02)	1.72	1.28	0.97	0.76
Cr	24	(8.0)	7.26	5.86	4.55	3.56	2.89	2.42	2.06	1.76	1.32	1.01	(0.80)
Mn	25	(7.7)	7.00	5.72	4.48	3.55	2.91	2.44	(2.08)	1.79	1.36	1.04	0.83
Fe	26	(7.4)	6.70	5.55	4.41	3.54	2.91	2.45	(2.11)	1.82	1.39	1.08	0.86
Co	27	(7.1)	6.41	5.41	4.34	3.51	2.91	2.46	(2.12)	1.84	1.42	1.11	0.89
Ni	28	(6.8)	6.22	5.27	4.27	3.48	2.90	2.47	(2.13)	1.86	1.46	1.14	0.92
Cu	29	(6.5)	6.00	5.11	4.19	3.44	2.88	2.46	2.13	1.87	1.47	1.16	(0.95)
Zn	30	(6.5)	5.84	5.00	4.14	3.42	2.88	2.47	2.14	1.88	1.48	1.18	0.96
Ga	31	(7.5)	6.70	5.62	4.51	3.64	3.00	2.53	2.18	1.91	1.50	1.20	0.98
Ge	32	(7.8)	6.89	5.93	4.81	3.87	3.16	2.63	2.24	1.94	1.51	1.22	0.99
As	33	(7.8)	6.99	6.05	5.01	4.07	3.32	2.74	2.31	1.99	1.54	1.23	1.01
Se	34	(7.7)	6.99	6.15	5.18	4.24	3.47	2.86	2.40	2.05	1.57	1.25	1.02
Br	35	(7.3)	6.80	6.15	5.25	4.37	3.60	2.97	2.49	2.12	1.60	1.27	1.04
Ag	47	(8.8)	8.24	7.47	6.51	5.58	4.75	4.05	3.46	2.97	2.22	1.70	1.35
W	74	(14)	—	11.80	—	7.43	—	5.16	—	3.85	2.99	2.39	1.96
Hg	80	(13.3)	12.26	10.82	9.18	7.70	6.48	5.50	4.72	4.09	3.16	2.51	2.05

Values in parentheses are interpolations or extrapolations.