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This Week's Citation Classic®

Hubbell J H, Veigele W J, Briggs E A, Brown R T, Cromer D T & Howerton R J. Atomic form factors, incoherent scattering functions, and photon scattering cross sections. *J. Phys. Chem. Ref. Data* 4:471-538, 1975; and Erratum. *J. Phys. Chem. Ref. Data* 6:615-6, 1977.

[Inst. Basic Standards, Natl. Bureau of Standards, Washington, DC; Kaman Sciences Corp., Colorado Springs, CO; Los Alamos Scientific Lab., Univ. California, NM; and Lawrence Livermore Lab., Univ. California, Livermore, CA]

This paper reviews available theoretical and measured atomic form factors and incoherent scattering functions and presents extended-range tables of these quantities for all neutral atoms $Z = 1$ to 100, plus bonded and molecular hydrogen. Integrated coherent (Rayleigh) and incoherent (Compton) scattering cross section tables are presented for photon energies 100 eV to 100 MeV. [The *SCI*® indicates that this paper has been cited in over 330 publications.]

X-Ray Scattering Data for Atoms

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Since the late 1940s, the Radiation Theory Group at the National Institute of Standards and Technology (formerly, the National Bureau of Standards [NBS]), initially under the leadership of Ugo Fano and more recently under Martin Berger, has been an internationally recognized source of photon and electron cross section and transport data. A brief history of the X-ray data project of this group was presented in an earlier *Citation Classic* commentary.[1]

This paper is highly cited because the presented data are required as input for a variety of radiation-interaction and atomic-physics computations needed in diverse medical, engineering, scientific, and analytical applications.

This publication draws together material from several sources, including previously unpublished work by the fifth author, Don Cromer. Don's earlier atomic form factor papers (see, e.g., reference 2) have become the standard references for nearly all X-ray crystallographic structure papers, with the result that Don has been identified as the most cited of all physics authors.[3] Tables based on the molecular hydrogen work of R.F. Stewart *et al.*,[4] another citation-rate superstar,[5] are also included in this work for convenience.

For producing tables of X-ray attenuation coefficients, coherent (Rayleigh) scattering and incoherent (Compton) scattering computations require as input the atomic form factor $F(x,Z)$ and incoherent scattering function $S(x,Z)$, respectively, where x is a momentum transfer variable and Z is the atomic number. Also, the latter are required for computations of the screening effects for electron-positron pair production in the field of the nucleus and in the field of the atomic electrons (triplet production), respectively. Pair and triplet production have thresholds of 1.02 MeV and 2.04 MeV, respectively.

The Cromer (and other available) values only covered the photon energy range of interest to crystallographers, up to about 30 keV for back angles. Bill Veigele and his assistant Edith Briggs persuaded Don to extend his calculations to encompass 1 MeV photons, for a 1973 Kaman Sciences compilation.[6]

For NBS compilations[7] extending well above 1 MeV, to 100 GeV, where "asymptopia" has essentially been reached, higher energy (corresponding to higher x-values) $F(x,Z)$ and $S(x,Z)$ values are needed. I used the behavior of the Bethe-Levinger relativistic K-shell formula to extrapolate beyond 1 MeV the Cromer-Veigele nonrelativistic values for $Z = 7$ to 100 and the R.T. Brown configuration-interaction values for $Z = 2$ to 6. Bob Howerton meticulously checked this pieced-together compilation for use in the widely distributed Livermore, Brookhaven, and Oak Ridge evaluated data sets for reactor shielding and other clientele.

The $S(x,Z)$ values in this paper, although nonrelativistic, are still the only extended-range systematic set available for high-energy photon interaction computation. However, attention is called to a set of relativistic Hartree-Fock-Slater modified $F(x,Z)$ values by D. Schaupp *et al.*,[8] which should be more accurate than those in this paper.

1. **Hubbell J H.** *Photon cross sections, attenuation coefficients, and energy absorption coefficients from 10 keV to 100 GeV.* Washington, DC: US Government Printing Office, August 1969. National Standard Reference Data Series Report No. NSRDS-NBS 29. 80 p. (Cited 400 times.) [See also: **Hubbell J H.** Citation Classic. (Thackray A, comp.) *Contemporary classics in the physical, chemical, and earth sciences.* Philadelphia: ISI Press, 1986. p. 54.]
2. **Cromer D T & Mann J B.** X-ray scattering factors computed from numerical Hartree-Fock wave functions. *Acta Crystallogr. Sect. A—Crys. Phys. Diffr. Theor. Gen. Crystallogr.* 24:321-4, 1968. (Cited 5,585 times.)
3. **Garfield E.** The 1,000 most-cited contemporary authors. Part 2A. Details on authors in the physical and chemical sciences and some comments about Nobels and academy memberships. *Essays of an information scientist.* Philadelphia: ISI Press, 1983. Vol. 5. p. 428-36.
4. **Stewart R F, Davidson E R & Simpson W T.** Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule. *J. Chem. Phys.* 42:3175-87, 1965. (Cited 7,815 times.) [See also: **Davidson E.** Citation Classic. (Barrett J T, ed.) *Contemporary classics in the life sciences. Volume 2: the molecules of life.* Philadelphia: ISI Press, 1986. p. 216.]
5. **Garfield E.** Most-cited articles of the 1960s. 1. Physical sciences. *Op. cit.*, 1981. Vol. 4. p. 156-66.
6. **Veigele W J.** Photon cross sections from 0.1 keV to 1 MeV for elements Z=1 to 94. *Atomic Data* 5:51-111, 1973. (Cited 275 times.)
7. **Hubbell J H, Gimm H A & Øverbø I.** Pair, triplet, and total atomic cross sections (and mass attenuation coefficients) for 1 MeV-100 GeV photons in elements Z=1 to 100. *J. Phys. Chem. Ref. Data* 9:1023-147, 1980. (Cited 40 times.)
8. **Schaupp D, Schumacher M, Smend F, Rullhusen P & Hubbell J H.** Small-angle Rayleigh scattering of photons at high energies: tabulations of relativistic HFS modified atomic form factors. *J. Phys. Chem. Ref. Data* 12:467-512, 1983. (Cited 20 times.)

14

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