

## Citation Classics

**Hanson H P, Herman F, Lea J D & Skillman S.** HFS atomic scattering factors. *Acta Crystallographica* **17**:1040-4, 1963.

**Atomic scattering factors calculated from Hartree-Fock-Slater (HFS) wave functions are presented for the neutral elements for  $Z = 2$  to  $Z = 100$  over a range of  $\sin \theta/\lambda$  values up to 6.0. It is asserted that this compilation should represent the most complete and accurate  $f$  values available. [The *SCI*<sup>®</sup> indicates that this paper was cited 1,079 times in the period 1961-1975.]**

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Dr. Harold P. Hanson  
Executive Vice President  
University of Florida  
Gainesville, Florida 32611

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“Naturally it is gratifying that a work that one has produced has become a Citation Classic. This means that the work has been useful and it has had a significant impact on the scientific scene.

“However, a paper that qualifies as a Citation Classic is not necessarily one which represents a major scientific break through. It is likely that most of the oft-cited papers are either (1) papers which outline a general method/technique that gets employed in numerous investigations or (2) papers which provide data, coefficients, parameters, etc.,

which are fundamental to a great number of experiments or studies. The paper I did with James Lea, Frank Herman, and Sherwood Skillman is in the latter category.

“The impact of the paper is in large part a result of timing. Herman and Skillman had just produced a generalized method of obtaining Hartree-Fock-Slater wave functions utilizing the newly-appreciated power of what was then the large computers. It was merely a matter of performing the indicated integration to produce a dense set of internally consistent atomic scattering factors for all elements of the periodic table. The wave functions themselves are of interest and significance to quantum theorists, but the atomic scattering factors have utility for a much wider group of investigators, viz., x-ray crystallographers, electron diffractionists, and even high-energy theorists.

“The question may be raised as to why these data continue to be used as extensively as they are at this late date. Atomic scattering factors which are presumably better have been produced in the meantime. However, the corrections to our numbers provided by more sophisticated wave functions are fairly small compared to the effects of bonding, geometry etc. It is still probably true that the Hanson-Herman-Lea-Skillman atomic scattering factors will give about as good experimental residuals as any other values that are generally available, and there is no impetus for investigators to change to other values.”