

the determination of the exact absorption correction difficult. The absorption factor varied from 0.16 for (002) to 0.51 for (020) amongst the inner reflexions, so that any error in it could mask the contribution of the hydrogen atom to the structure factors. Another cause could be the inaccuracies of the data arising from systematic errors in intensity measurement and scaling. The method of scaling the three-dimensional data necessitated frequent rescaling in the course of the refinement.

From an examination of all the O-O distances in the structure, however, it is clear that there is an intermolecular hydrogen bond, since the O(1)2-O(3) contact (Table 3) is  $2.514 \pm 0.011$  Å long, whilst the two next shortest O-O contacts for oxygen atoms not in the same carboxyl group are 2.98 and 3.11 Å. This intermolecular hydrogen bond means that because of the double nature of the anion the strain in the anion is so great that the ion is neither planar nor has an internal hydrogen bond.

We wish to express our gratitude to Prof. H. Lipson for his constant interest. All the computations were performed on the Mercury Computer of the Manchester University Computing Laboratory and we take great pleasure both in thanking Prof. F. C. Williams for extending this facility to us and in thanking those who have let us use their programs. One of us (S. K. K.) would also like to express thanks to the Principal and the Governing Body of the Hans Raj College, Delhi, India for the granting of study leave and to the British Council for providing the travel grant under the Commonwealth University Interchange Programme.

*Acta Cryst.* (1965). **18**, 104

## Scattering Factors Computed from Relativistic Dirac-Slater Wave Functions\*

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(Received 24 February 1964)

Scattering factors for a total of 208 neutral atoms, positive ions and a few negative ions are given in tabular form and as nine-parameter analytic functions. These scattering factors have been computed from relativistic self-consistent field wave functions which include Slater's approximate exchange correction.

### Introduction

Two extensive tabulations of scattering factors have recently been published. Hanson, Herman, Lea &

\* Work performed under the auspices of the U.S. Atomic Energy Commission.

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Skillman (1964) have computed, for neutral elements from  $Z=1$  to  $Z=100$ , scattering factors based on self-consistent field Hartree-Fock-Slater (HFS) wave functions which had been computed by Herman & Skillman (1963). For these wave functions, Slater's (1951) approximate  $\rho^{\frac{1}{2}}$  method rather than Fock's



SCATTERING FACTORS FROM DIRAC-SLATER WAVE FUNCTIONS

Table I (cont.)

Table with 16 columns: S, MR, MR-1, KR, RB, RB+1, SR, SR+2, Y, Y+3, ZR, ZR+4, NB, NB+3, NB+5, MC, MD+3. Rows range from 0. to 2.00.

Table with 16 columns: S, MD+5, PD+6, TO, RU, MU+3, RH, RH+3, RH+4, PD, PC+2, PC+4, AG, AG+1, AG+2, CD. Rows range from 0. to 2.00.

Table with 16 columns: S, CD+2, IN, IN+3, SN, SN+2, SN+4, SB, SB+3, SB+5, TE, I, I-1, XE, CS, CS+1, BA. Rows range from 0. to 2.00.

Table with 16 columns: S, BA+2, LA, LA+3, CE, CE+3, CE+4, PR, PR+3, PR+4, ND, ND+3, PP, PP+3, SP, SP+3, EU. Rows range from 0. to 2.00.

Table 1 (cont.)

Table with 18 columns: S, EU+2, EU+3, GC, GD+3, TB, TB+3, DY, DY+3, HO, HO+3, ER, ER+3, TH, TH+3, YB, YB+2. Rows range from 0.0 to 2.00.

Table with 18 columns: S, YB+3, LU, LU+2, HF, HF+4, TA, TA+5, M, M+6, RE, OS, OS+4, IR, IR+3, IR+4, PT. Rows range from 0.0 to 2.00.

Table with 18 columns: S, PT+2, PT+4, AU, AU+1, AU+3, HG, HG+1, HG+2, IL, IL+1, IL+5, PB, PB+2, PB+4, S1, B1+3. Rows range from 0.0 to 2.00.

Table with 18 columns: S, B1+5, PG, AT, RN, FR, KA, AC, AC+5, TH, TH+4, PA, U, U+3, U+4, U+6, NP. Rows range from 0.0 to 2.00.

SCATTERING FACTORS FROM DIRAC-SLATER WAVE FUNCTIONS

Table 1 (cont.)

Table with columns S, NP+3, NP+4, NP+6, PU, PU+3, PU+4, PU+6, AM, AM+3, CM, BK, CF, ES, FM, MU, NO. Rows include numerical data for various scattering factors.

Table 2. Coefficients for nine-parameter analytic fit of Dirac-Slater scattering factors in the range 0 <= s <= 2.0 A^-1

Large table with columns A1-C1, A10-C10, A11-C11, A12-C12, A13-C13, A14-C14, A15-C15, A16-C16, A17-C17, A18-C18, A19-C19, A20-C20. Rows include coefficients for various elements and parameters.

method was used to incorporate exchange. Cromer, Larson & Waber (1963, 1964), using self-consistent field Hartree ( $H$ ) wave functions computed by Boyd, Larson & Waber (1965), have computed scattering factors for elements from  $Z=2$  to  $Z=98$  and for many of the chemically significant positive ions.

The  $HFS$  scattering factors ought to be more accurate than the  $H$  scattering factors because the former include an approximate exchange correction. Both, however, will be in error for the heavy elements because relativistic effects have not been accounted for.

Lieberman, Waber & Cromer (1965) have made extensive self-consistent field calculation of relativistic wave functions by using the Dirac equations with Slater's (1951) approximate exchange correction. These wave functions have been called Dirac-Slater ( $DS$ ) wave functions and are the relativistic equivalent of the  $HFS$  wave functions. Although not many comparisons can be made because of the scarcity of relativistic calculations, Lieberman *et al.* (1965) have shown that the eigenvalues for these  $DS$  wave functions are in better agreement with experimental X-ray levels than are any other published values.

Scattering factors for a total of 208 neutral atoms, positive ions and a few negative ions have been computed from the  $DS$  wave functions and are presented here. For the heavy atoms and ions these scattering factors should be more accurate than any that have been previously available.

These  $DS$  wave functions have also been used to compute anomalous dispersion corrections for five commonly used X-ray wavelengths (Cromer, 1965).

### Calculations

Details of the self-consistent field wave function calculations have been given by Lieberman *et al.* (1965). A logarithmic scale of radii was used and the radial domain extended from  $1.056 \times 10^{-4}$  to 60.0 Bohr units. This range was divided into 420 intervals equally spaced with  $\Delta \ln r = 1/32$ . The scattering factors were computed with an IBM 7094 computer, from the total electronic radial density by straightforward means (James, 1948). Calculations were made at 201 points in the range  $s_x = \sin \theta / \lambda$  from 0 to  $2.00 \text{ \AA}^{-1}$  at intervals of  $0.01 \text{ \AA}^{-1}$ . Also, at 19 points within this range, the individual orbital transforms were computed from the single-electron densities. These orbital transforms and the total scattering factors at the 201 points have been published in a Los Alamos Scientific Laboratory report (Cromer & Waber, 1964).

### Explanation of the tables

The results are given here in two forms. Table 1 lists the values of  $f$  as a function of  $s_x$  at the intervals used in *International Tables for X-ray Crystallography* (1959). Table 2 gives the coefficients  $a_i$ ,  $b_i$  and  $c$  which fit the function

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

for  $n=4$ . This analytical function is a concise means of expressing the  $f$  curves over the entire range and also is a convenient means for entering the  $f$  curves into a computer. The analytic fit is a weighted fit, as done by Forsyth & Wells (1959), so that the curve is fitted best at  $s_x = 0.5 \text{ \AA}^{-1}$ . The last column in Table 2 gives the quantity

$$E = \frac{100}{f(0)} \left[ \frac{\sum w_i \delta_i^2}{\sum w_i} \right]^{\frac{1}{2}}$$

which is the error of the fit expressed as a percentage of the scattering factor at  $s_x = 0$ . The analytic fit is in general very good.

A comparison of the scattering factors obtained from the four different atomic models for which extensive scattering factors exist (Hartree, Hartree-Fock-Slater, Dirac-Slater and Thomas-Fermi-Dirac) will be the subject of a future paper.

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