situated, within experimental error, on the $O \cdots O$ connecting lines between neighboring molecules. The only important differences between the 1934 and 1953 results are in the location of the hydrogen atoms and in the bond angles $B–O \wedge O–H \cdots O$ and $B–O \wedge O \cdots H–O$, as the following comparison shows:

	1934	1953 (Mean values)
B–O	1·36 Å	1·361 Å
$O–H \cdots O$	2·71 Å	2·720 Å
O–H	1·36 Å	0·88 Å
$O \cdots H$	1·36 Å	1·84 Å
$B–O \wedge O–H \cdots O$	120°	113·9°
$B–O \wedge O \cdots H–O$	120°	126·1°

The observed value of 0·88 Å is about 0·1 Å smaller than anticipated. This is probably due to the fact that spherically symmetrical oxygen atoms were assumed in the procedure used to deduce the hydrogen positions. Presumably there is an excess of electron density in the oxygen atom near the hydrogen atom, and by the assumed spherical symmetry for oxygen this excess density is inappropriately assigned to hydrogen, resulting in an apparent displacement of the hydrogen towards the oxygen atom.

The layers are not perfectly plane as was concluded in 1934. However, the displacements out of the plane $z = \frac{1}{4}$ are very small, amounting to a maximum value of 0·11 Å for the O_{VI} atom. The idealized layers $z = \frac{1}{4}$ and $\frac{3}{4}$ are 3·181 Å apart, so that only weak bonds exist between layers, in agreement with the observed perfect basal cleavage.

The layers are stacked in such a manner that a number of oxygen atoms are approximately below or above boron and hydrogen atoms of neighboring layers. The shortest $B \cdots O$ distances between layers are 3·157 Å ($B_{II} \cdots O_{II}$) and 3·184 Å ($B_{I} \cdots O_{V}$). It appears that these boron–oxygen interactions dominate the hydrogen–oxygen interactions between layers in determining the actual values of the angles α_1 and α_2. And it seems also that the small tilts of the BO_3-groups relative to the plane (001) are mainly due to the interactions between boron and oxygen atoms.

Were all atoms situated exactly at $z = \frac{1}{4}$ without interaction between layers, then perfect trigonal symmetry should prevail in a layer. The small departure from trigonal symmetry actually observed (a_1 and a_2 differing by 0·2%, $\alpha_3 = 119{\cdot}83°$ instead of 120°) is indeed a direct consequence of the small tilts of the BO_3-groups relative to the plane $z = \frac{1}{4}$ caused by weak interaction between layers.

The help given by Miss Anne Plettinger in making some of the intensity measurements is gratefully acknowledged. Most of the Fourier syntheses used in the investigation were carried out with the aid of XRAC during three separate visits to Pennsylvania State College. Prof. Raymond Pepinsky is sincerely thanked for his hospitality and generosity in making XRAC available to the writer. The writer is also indebted to the XRAC staff members for the help they have given.

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On the Completion and Extension of the Table of Atomic Scattering Factors Published by Viervoll & Ögrim

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The table of atomic scattering factors (based on the Hartree self-consistent field) published by Viervoll & Ögrim has a gap between calcium ($Z = 20$) and chromium ($Z = 24$). This gap has been bridged by calculating the screening parameter for the ($3d$) electron in $Ca^{+}(3d)$. This calculation has been done by a new method, which has possibilities for use with heavier atoms. The atomic scattering factors for scandium to vanadium are tabulated as functions of $s = 4\pi(\sin\theta)/\lambda$.

Viervoll & Ögrim (1949) have published a revised table of atomic scattering factors, up to atomic number 29 (copper), based on recent calculations of the Hartree self-consistent field for a number of atoms. The metals scandium, titanium and vanadium, however, are omitted from this table because of the uncertain extrapolation of the screening parameters for the ($3d$) electrons. In working on the structures of the mineral vanadates (Barnes & Qurashi, 1952; Qurashi

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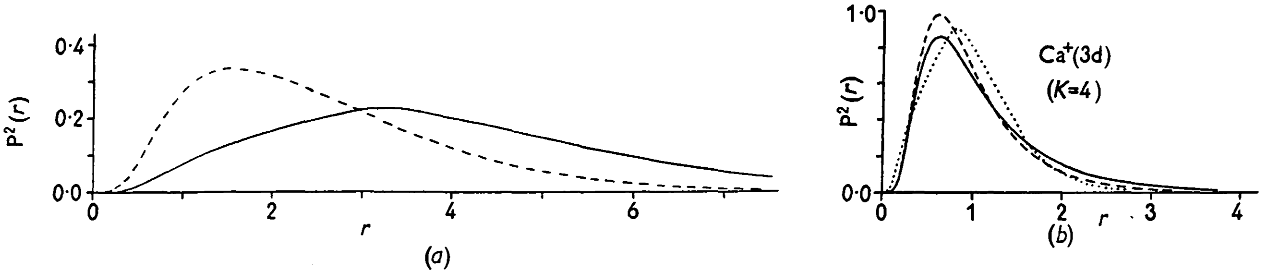

Fig. 1. Curves for the radial density, $P^2(r)$, of the $(3d)$ electron as a function of the radius r (in atomic units). Full line: without exchange; broken line: with exchange.
(a) Ca^+ $(3d)$. (b) Cu^+ $(3d)$; dotted line: Ca^+ $(3d)$ with scale factor, K, equal to 4·0.

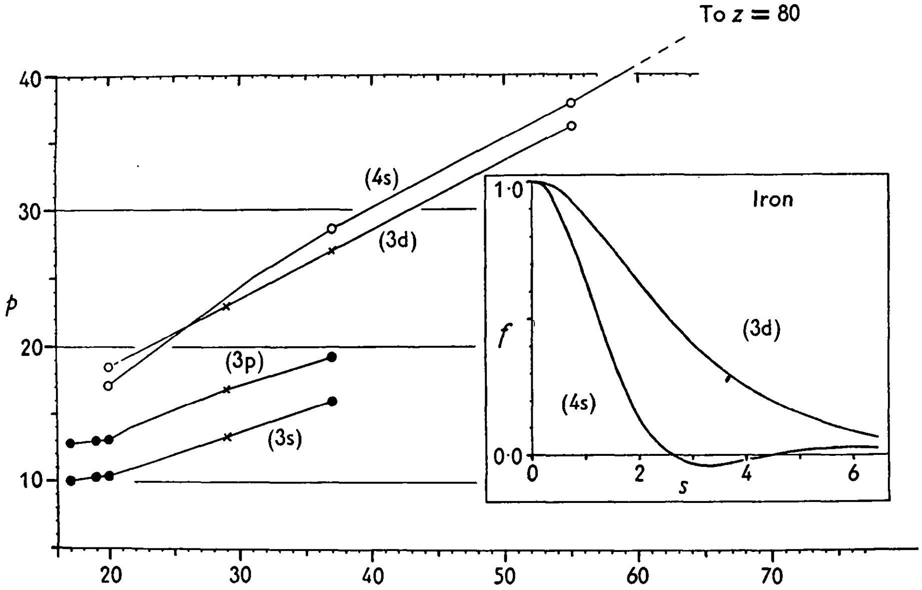

Fig. 2. Plots of screening parameters (p) against atomic number (Z) for some electronic sub-shells. ●: James & Brindley; ×: Viervoll & Ögrim; ○: author. Inset: comparison of the contributions of one $(3d)$ and one $(4s)$ electron to the scattering factor of iron.

& Barnes, 1953), a need has been felt for scattering factors for V, Zn, As, etc. more accurate than those given by the Thomas–Fermi values, which are apt to be seriously in error for these atoms.

A search of the literature has shown that self-consistent field calculations (both with and without exchange) are available for the excited $(3d)$ state of Ca^+ (Hartree & Hartree, 1938). With the addition of one $(4s)$ electron, this would become the $(3d)$ $(4s)$ state of neutral calcium, which is comparable with the normal $(3d)^{10}$ $(4s)$ state of copper. Since in the plot of screening parameter (p) against atomic number (Z), Viervoll & Ögrim have used the screening parameter for Cu^+ $(3d)^{10}$, it seems reasonable to use the value for Ca^+ $(3d)$ to fix the lowest point on the plot for the $(3d)$ sub-shell.

Fig. 1(a) shows the curves for radial density $[U(r) = P^2(r)]$ plotted against r for the $(3d)$ electron of Ca^+ $(3d)$, and Fig. 1(b) shows the corresponding curves for Cu^+. For uniformity with Viervoll & Ögrim's calculations, we shall neglect the effects of exchange; it is interesting to note, however, that the *total* effect of exchange on the scattering factor for the $(3d)$ electrons is approximately doubled in going from scandium to copper. James & Brindley (1931) have shown that to a good approximation the radial density curves (and the f-curves) for a given sub-shell differ only by a scale factor proportional to $(Z-p)$. Thus, we have

$$(Z-p)_{\mathrm{Cu}}/(Z-p)_{\mathrm{Ca}} = K \qquad (K > 1)\,, \tag{1}$$

where K is the scale factor required to bring the curves into best coincidence. This can be done by directly comparing the radial density curves, and we get $K \simeq 4$ (cf. Fig. 1(b)). Although the two curves cannot be made to agree completely, it is easily seen that the value of K obtained is correct to within 10% approximately, so that we can take the value of K as $4{\cdot}0 \pm 0{\cdot}4$, and get

$$(Z-p)_{\mathrm{Ca}^{+}\,(3d)} = \frac{1}{K}(Z-p)_{\mathrm{Cu}^{+}\,(3d)} = 6{\cdot}0/4{\cdot}0 = 1{\cdot}50 \pm 0{\cdot}15\,,$$

whence

$$(p)_{\mathrm{Ca}^{+}\,(3d)} = 18{\cdot}50 \pm 0{\cdot}15.^{*} \qquad (2)$$

This value agrees with the linearly extrapolated value, 18·50 (cf. Fig. 2); we can therefore retain unchanged the calculations of Viervoll & Ögrim for the atoms chromium to nickel. The scattering factors for scandium, titanium and vanadium have now been calculated, and are given in Table 1 for integral values of $s = 4\pi\,(\sin\theta)/\lambda$. Check calculations for chromium gave a mean deviation of less than 0·02 units from Viervoll & Ögrim's results.

Table 1. *Calculated scattering factors for integral values of* $s = 4\pi\,(\sin\theta)/\lambda$.

$\frac{4\pi \sin\theta}{\lambda}$	Sc	Ti	V
$\times 10^8$			
0	21·00	22·00	23·00
1	17·83	18·71	19·71
2	15·56	16·23	17·11
3	13·27	13·84	14·62
4	11·33	11·82	12·47
5	9·81	10·27	10·81
6	8·67	9·06	9·49
7	7·88	8·16	8·51
8	7·28	7·53	7·81
9	6·76	7·01	7·26
10	6·32	6·56	6·78
11	5·92	6·17	6·37
12	5·55	5·80	6·00
13	5·20	5·46	5·67
14	4·84	5·12	5·36
15	4·49	4·78	5·05
16	4·16	4·46	4·73
17	3·86	4·15	4·44
18	3·58	3·88	4·14
19	3·32	3·61	3·89
20	3·08	3·36	3·62
21	2·88	3·15	3·39
22	2·68	2·94	3·18
23	2·50	2·74	2·99
24	2·34	2·56	2·81
25	2·21	2·41	2·63
26	2·08	2·27	2·47
27	1·98	2·15	2·33
28	1·90	2·04	2·21
29	1·82	1·94	2·09
30	1·74	1·87	2·00

The (4*s*) *electrons*.—These have been neglected (except for $s = 0$) in Viervoll & Ögrim's table, and (for uniformity) also in the present Table 1. However, a plot of the $f(s)$ curves (Fig. 2 (inset)) shows that in the significant range ($s \equiv 4\pi\,(\sin\theta)/\lambda < 2$) the contribution of two (4*s*) electrons in the transition group is of the same order as that of one (3*d*) electron and should therefore be included. A standard scattering-factor curve for the (4*s*) electrons has been calculated from Ca, Rb^{+} and Cs^{+} data (Hartree & Hartree, 1935; Hartree, 1934, 1935), and screening parameters (Fig. 2) have been derived. The inset in Fig. 2 shows the contributions to f from a (3*d*) and a (4*s*) electron of iron. A complication caused by the (4*s*) electrons is that the (4*s*) and (3*d*) electron densities overlap—considerably so for scandium. This introduces an extra electrostatic screening for the (3*d*) electrons, thus lowering the value of $(Z-p)_{3d}$. It is not difficult to show that the change in $(Z-p)$ is of the order of 0·3 for scandium; it decreases as Z increases, but the net effect on the scattering factor for the (3*d*) subshell remains about the same, because of the increasing number of the (3*d*) electrons.

The author is indebted to Dr W. H. Barnes and to Prof. R. Pepinsky for their interest.

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* The limits of error ($\pm 0{\cdot}15$) are satisfactory in this particular case. In general, however, considerably greater accuracy is obtainable by using (in place of $U(r)$) a function $\varphi(s) \simeq \int_0^{1\cdot 7/s} U(r)dr$. Details of this will be given in a later paper, wherein it is proposed to extend the (self-consistent field) scattering-factor calculations to atoms heavier than copper.