if, for example, we had a tetragonal crystal and a subset of three relations among six q numbers. For this subset we would necessarily find at least three independent q numbers, whereas actually only two are needed. If we solved for three of the q numbers in terms of the remaining three and then substituted these results in the remaining relations, they would necessarily be satisfied. We might then erroneously conclude that the crystal was orthorhombic. In the example worked out above, using this short procedure we found two independent q numbers (confirmed by the full procedure). We might have been in error when we called the crystal tetragonal or hexagonal. It conceivably could be cubic on the basis of the subset of three relations with only one of the q numbers being linearly independent. This would require that a linear dependence relation exist between q_1 and q_2 of the form $m_1q_1 = m_2q_2$. Since no such relation exists, the short procedure was valid in this case.

In seeking the additional relations among the q numbers needed for the linear dependence test, tables were prepared of: (*a*) multiples of the q's up to $10q$; (*b*) $q_{k+1}-q_k$; (*c*) $q_{k+2}-q_k$; (*d*) $q_{k+3}-q_k$; (*e*) $q_{k+4}-q_k$; (*f*) $2q_{k+1}-q_k$, etc. The next step consists in examining these tables for numbers which are equal within the permitted limits of error. For the present purpose this limit was set at 0·0003 in $\sin^2\theta$. If the limit is not made so small, accidental equalities of a spurious nature will be listed and the procedure will fail. As Hesse has stated, the use of focusing cameras is almost a necessity.

The relation $7q_1+q_6-2q_7 = 0$ (0·0003) was found by noting that the quantity $2q_7-q_6$ was equal to $7q_1$. The relation $q_3-q_4-q_6+q_8+q_9-q_{10} = 0$ (0·0000) was found by noting that $(q_{10}-q_9)+(q_4-q_3) = (q_8-q_6)$. Similarly $2(q_8-q_6) = q_5$ becomes $q_5+2q_6-2q_8 = 0$ (0·0000). The equality $(q_{11}-q_9) = 2(q_3-q_2)+(q_9-q_8)$ becomes $2q_2-2q_3+q_8-2q_9+q_{11} = 0$ (0·0001). It is possible to guard against spurious relations by cross checking to see whether they imply relations which are not of the desired precision. Thus the relation (spurious) $q_8-q_6 = q_7-q_5$ (0·0004) was rejected because of the relation $2(q_8-q_6) = q_5$ (0·0000). These relations, if both correct, taken together require $2(q_8-q_6) = 2(q_7-q_5)$, or $2q_7 = 3q_5$. The latter is not correct since $2q_7 = 0{\cdot}8722$, while $3q_5 = 0{\cdot}8730$, the difference 0·0008 being far outside the acceptable range. The rejection of $q_8-q_6 = q_7-q_5$ also implies rejection of $q_8-q_7 = q_6-q_5$.

It must be emphasized that the selection of these relations must be done with care, since this is the only point in the procedure at which observational or subjective errors enter. The outcome of the remainder of the procedure is completely dependent on the care used at the start.

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An Extended Table of Atomic Scattering Factors

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A table of atomic scattering factors is given for the elements H to Cu for values of $(4\pi \sin\theta)/\lambda$ up to 30.

In applying the sector method of electron diffraction (Viervoll, 1947) we have for some time made use of new tables of atomic scattering factors, f, which cover a greater range of $(\sin\theta)/\lambda$ than the corresponding tables used by the X-ray crystallographers. Our f values (Table 2) are given as functions of $s = (4\pi \sin\theta)/\lambda$ (A.$^{-1}$), where θ is the Bragg angle.

The calculations of the f values are mainly based on those of James & Brindley (1931), who give the functions for values of s up to about 14. We have extended the s range to 30. For our purpose we did not find it necessary to apply wave functions 'with exchange' which would introduce very small effects for higher s values. These effects would be somewhat greater for smaller s values (Brindley & Ridley, 1938), but may still be assumed to be without significance for ordinary structure determinations.

The atomic scattering factor may be considered as a sum of electronic scattering factors, each of which corresponds to an electron of the atom. James & Brindley found that a suitable linear transformation of the s scales could bring the scattering factors of the same electron group (same n and l) in different atoms to coincide very closely.

We have found that the differences between these curves would produce a difference in the f curves of the same order of magnitude as the probable error due to numerical calculations, and we have therefore used a mean of the transformed curves in our calculations (Table 1). By this procedure our f curves assume a somewhat smoother form than those of James & Brindley. This is of importance when applied in connexion with the sector method of molecular structure determinations, as false 'humps' in the f curves have great influence on the radial distribution functions.

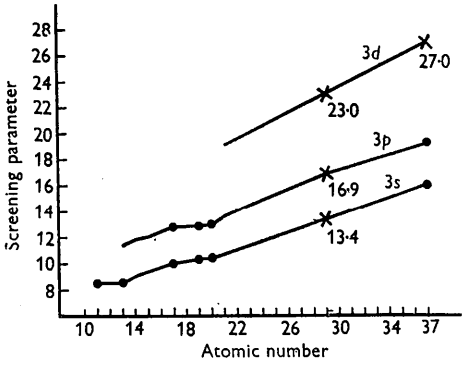

Fig. 1. Screening parameters of the 3s, 3p and 3d electrons. ● Values given by James & Brindley. × Values obtained by us.

In the evaluation of these mean curves we have included calculations based on the electron distribution of Na^+ (Fock & Petrashen, 1934), O (Hartree, Hartree & Swirles, 1939), K^+ (Hartree, 1934), and Cu^+ (Hartree, 1933). The numerical calculations, the difficulties of which increase with higher s values, have been performed by different methods to secure sufficient accuracy.

The values of the 'screening parameters', which are introduced by the linear transformations, differ slightly from those used by James & Brindley for the 3s, 3p and 3d electrons of atoms with numbers greater than 20 (Fig. 1). This is owing to the use made of the electron distribution of Cu^+, which was not available at the time when James & Brindley made their calculations. We believe therefore, that our f values are more accurate than those of James & Brindley for atomic numbers greater than 20.

This has also been checked by an independent calculation based on the complete electron distribution of Cu^+. The differences between the values obtained in this way and the table-values occur only in the second decimal. This indicates that the probable error, due to our method of calculation and interpolation, is smaller than 0·1.

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Table 1. *Mean of the transformed electronic scattering factors*

$\frac{s}{Z-p}$	1s	2s	2p	3s	3p	3d
0	1·000	1·000	1·000	1·000	1·000	1·000
0·1	1·000	0·978	0·980	0·936	0·954	0·967
0·2	0·998	0·922	0·935	0·746	0·813	0·894
0·3	0·992	0·836	0·866	0·522	0·631	0·790
0·4	0·982	0·729	0·781	0·315	0·453	0·677
0·5	0·971	0·612	0·694	0·143	0·298	0·570
0·6	0·956	0·497	0·600	0·039	0·188	0·469
0·7	0·938	0·389	0·509	0·000	0·103	0·376
0·8	0·919	0·296	0·427	−0·027	0·046	0·300
0·9	0·897	0·217	0·353	−0·029	0·009	0·244
1·0	0·871	0·155	0·290	−0·021	−0·008	0·199
1·2	0·820	0·057	0·194	+0·007	−0·017	0·117
1·4	0·764	0·012	0·126	0·020	−0·008	0·073
1·6	0·704	−0·008	0·079	0·021	+0·010	0·038
1·8	0·648	−0·014	0·050	0·019	0·021	0·018
2·0	0·592	−0·013	0·032	0·011	0·025	0·003
2·5	0·474	−0·001	0·004	0·000	0·024	−0·009
3·0	0·370	+0·012	−0·006	—	0·015	−0·011
3·5	0·284	0·018	−0·006	—	0·008	−0·010
4·0	0·218	0·020	−0·005	—	0·004	−0·007
5·0	0·134	0·018	−0·003	—	0·000	0·000
6·0	0·079	0·013	−0·001	—	—	—
8·0	0·040	0·006	0·000	—	—	—
10·0	0·020	0·004	—	—	—	—
12·0	0·008	0·000	—	—	—	—

Z is the atomic number, p the screening parameter.

Table 2. *Atomic scattering factors*

$\frac{4\pi}{\lambda}\sin\theta$	H	Li	Be	B	C	N	O	F	Na	Mg	Al	Si
$\times 10^8$												
0	1·000	3·00	4·00	5·00	6·00	7·00	8·00	9·00	11·00	12·00	13·00	14·00
1	0·874	2·34	3·21	3·92	5·07	6·29	7·44	8·41	9·97	10·83	11·30	12·03
2	0·611	1·87	2·24	2·72	3·57	4·85	6·17	7·09	8·76	9·18	9·70	10·04
3	0·374	1·68	1·84	2·09	2·59	3·54	4·77	5·55	7·65	8·04	8·49	8·77
4	0·223	1·49	1·67	1·81	2·07	2·69	3·62	4·25	6·40	7·05	7·51	7·92
5	0·133	1·29	1·55	1·67	1·82	2·16	2·85	3·31	5·26	6·02	6·58	7·10
6	0·081	1·09	1·42	1·56	1·67	1·89	2·35	2·67	4·29	5·05	5·70	6·28
7	0·051	0·93	1·28	1·44	1·58	1·71	2·00	2·23	3·56	4·23	4·88	5·49
8	0·034	0·77	1·14	1·36	1·50	1·59	1·81	1·98	2·99	3·58	4·19	4·77
9	0·023	0·63	1·02	1·25	1·41	1·52	1·66	1·80	2·54	3·06	3·65	4·14
10	0·016	0·51	0·90	1·15	1·33	1·44	1·55	1·66	2·24	2·66	3·13	3·62
11	0·011	0·43	0·79	1·05	1·24	1·36	1·46	1·55	2·02	2·35	2·74	3·17
12	0·008	0·36	0·68	0·95	1·16	1·29	1·38	1·47	1·86	2·11	2·44	2·82
13	0·007	0·30	0·59	0·86	1·08	1·21	1·32	1·41	1·72	1·94	2·20	2·53
14	0·005	0·25	0·51	0·77	1·00	1·14	1·25	1·35	1·62	1·81	2·03	2·31
15	0·004	0·20	0·44	0·69	0·92	1·08	1·19	1·30	1·52	1·69	1·88	2·11
16	0·003	0·16	0·39	0·61	0·85	1·02	1·13	1·24	1·44	1·59	1·77	1·96
17	0·002	0·14	0·34	0·54	0·77	0·95	1·07	1·19	1·36	1·51	1·67	1·84
18	0·002	0·13	0·30	0·49	0·70	0·89	1·02	1·14	1·30	1·43	1·58	1·74
19	0·002	0·11	0·26	0·44	0·64	0·83	0·96	1·09	1·26	1·35	1·50	1·64
20	0·001	0·10	0·22	0·39	0·58	0·77	0·91	1·04	1·21	1·30	1·42	1·56
21	0·001	0·09	0·19	0·35	0·53	0·70	0·85	1·00	1·17	1·24	1·36	1·49
22	0·001	0·08	0·16	0·32	0·48	0·65	0·81	0·95	1·12	1·20	1·29	1·42
23	0·001	0·07	0·15	0·29	0·44	0·60	0·75	0·90	1·08	1·16	1·24	1·36
24	0·001	0·06	0·13	0·26	0·41	0·55	0·70	0·86	1·04	1·12	1·20	1·30
25	0·001	0·05	0·12	0·23	0·37	0·51	0·66	0·81	1·00	1·08	1·16	1·24
26	0·000	0·04	0·11	0·21	0·34	0·47	0·61	0·76	0·97	1·05	1·12	1·20
27	0·000	0·04	0·10	0·18	0·31	0·44	0·57	0·72	0·93	1·01	1·09	1·16
28	0·000	0·03	0·09	0·16	0·29	0·41	0·53	0·67	0·90	0·98	1·05	1·13
29	0·000	0·03	0·08	0·14	0·26	0·38	0·50	0·63	0·86	0·94	1·02	1·09
30	0·000	0·02	0·08	0·13	0·24	0·35	0·46	0·59	0·83	0·91	0·99	1·06

$\frac{4\pi}{\lambda}\sin\theta$	P	S	Cl	K	Ca	Cr	Mn	Fe	Co	Ni	Cu
$\times 10^8$											
0	15·00	16·00	17·00	19·00	20·00	24·00	25·00	26·00	27·00	28·00	29·00
1	13·17	14·24	15·35	16·98	17·21	21·40	21·72	22·80	23·88	24·96	26·97
2	10·72	11·50	12·39	14·54	14·52	18·35	19·01	20·15	21·31	22·50	24·42
3	9·14	9·63	10·21	12·11	12·91	15·50	16·25	17·30	18·40	19·63	21·34
4	8·20	8·50	8·80	10·24	10·97	13·17	13·86	14·79	15·81	16·84	18·39
5	7·50	7·75	7·99	8·83	9·47	11·35	11·97	12·72	13·55	14·52	15·82
6	6·75	7·12	7·36	7·95	8·34	9·93	10·49	11·14	11·79	12·58	13·66
7	6·04	6·46	6·82	7·29	7·61	8·87	9·29	9·83	10·41	11·10	11·88
8	5·35	5·84	6·26	6·74	7·00	8·07	8·40	8·83	9·27	9·87	10·59
9	4·70	5·18	5·69	6·25	6·50	7·49	7·83	8·07	8·41	8·90	9·48
10	4·13	4·64	5·13	5·83	6·04	6·99	7·24	7·49	7·78	8·12	8·58
11	3·64	4·13	4·61	5·42	5·66	6·57	6·78	7·02	7·26	7·55	7·90
12	3·22	3·68	4·14	4·97	5·28	6·19	6·41	6·60	6·81	7·06	7·36
13	2·88	3·27	3·73	4·56	4·88	5·86	6·06	6·24	6·44	6·64	6·88
14	2·60	2·94	3·35	4·19	4·51	5·58	5·74	5·92	6·10	6·23	6·47
15	2·37	2·67	3·02	3·84	4·17	5·29	5·47	5·62	5·80	5·96	6·14
16	2·17	2·45	2·73	3·51	3·86	4·99	5·20	5·38	5·52	5·68	5·83
17	2·03	2·26	2·51	3·22	3·56	4·69	4·92	5·12	5·29	5·43	5·57
18	1·90	2·10	2·32	2·95	3·29	4·41	4·65	4·85	5·04	5·20	5·33
19	1·81	1·97	2·17	2·70	3·04	4·15	4·38	4·59	4·79	4·97	5·12
20	1·70	1·85	2·03	2·50	2·81	3·89	4·14	4·35	4·55	4·73	4·89
21	1·62	1·76	1·92	2·32	2·59	3·65	3·90	4·13	4·32	4·51	4·66
22	1·54	1·68	1·81	2·16	2·43	3·42	3·66	3·90	4·10	4·28	4·45
23	1·47	1·60	1·73	2·04	2·27	3·22	3·45	3·68	3·90	4·07	4·25
24	1·41	1·53	1·66	1·94	2·13	3·02	3·25	3·48	3·68	3·88	4·05
25	1·35	1·46	1·58	1·84	1·99	2·84	3·07	3·29	3·50	3·69	3·86
26	1·29	1·40	1·52	1·76	1·91	2·67	2·89	3·12	3·31	3·51	3·68
27	1·24	1·35	1·45	1·69	1·81	2·52	2·72	2·95	3·14	3·34	3·51
28	1·20	1·30	1·40	1·62	1·74	2·38	2·57	2·78	2·98	3·18	3·35
29	1·16	1·25	1·35	1·56	1·67	2·26	2·44	2·63	2·82	3·03	3·20
30	1·12	1·21	1·30	1·50	1·61	2·16	2·32	2·50	2·67	2·87	3·06