others may be allowed to vibrate independently. The **T** and **ω** tensors of the several rigid units are refined directly, as in Pawley's method, along with the usual coordinates, occupancy factors, *etc.* Experience suggests that this one-stage procedure may be highly advantageous, especially in rate of convergence, provided the molecules are sufficiently rigid and the f curves used (for X-ray data) represent the stationary-atom electron densities to the required accuracy. When these conditions are not met, the two-stage procedure, or a comparison of the two, may help to reveal inadequacies of the model, due to internal vibrations, charge polarization, altered hybridization, *etc.*, more readily than extensive difference syntheses.

The tensor formulation is also useful for evaluation of the libration corrections to the atomic coordinates. Assuming for simplicity that our refinement procedure has located the centroids of the atomic peaks rather than their maxima (either assumption is an approximation requiring justification in particular circumstances), we may, for the present argument, disregard the factor $D(a\varphi)$ in Cruickshank's (1961) equation (6) and obtain from his equations (10) the matrix equation for the coordinate shifts, in an orthonormal system,

$$-[\varepsilon_\lambda\varepsilon_\mu\varepsilon_\nu]=\tfrac{1}{2}\{t[\lambda\mu\nu]-[\lambda\mu\nu][\omega]\}\ ,$$

where t is the trace of $[\omega]$. The tensor analog of this equation, valid in any coordinate system, gives the corrected atomic coordinates

$$\lambda^k-\varepsilon^k=(1+\tfrac{1}{2}t)\lambda^k-\tfrac{1}{2}\lambda^i\omega_i^k\ .$$

Here, λ^k are the uncorrected coordinates, measured from the center of libration; the mixed covariant-contravariant components of **ω** may be evaluated as

$$\omega_i^k=\omega_{ij}G^{jk}\ ,$$

where the matrix $[G^{jk}]$ is inverse to $[G_{ij}]$; and the trace

$$t=\sum_i \omega_i{}^i$$

is invariant under all coordinate transformations.

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The anisotropic temperature factor of atoms in special positions.

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(*Received* 3 *April* 1965 *and in revised form* 20 *September* 1965)

In this paper a table of symmetry restrictions on anisotropic temperature factor parameters for all special positions of the 230 space groups is presented. The text explains the table and describes the computer program which was used to derive it. The relationships between the various restricted forms are displayed diagrammatically. No recommendations for the method of programming these restrictions in least-squares refinement are included.

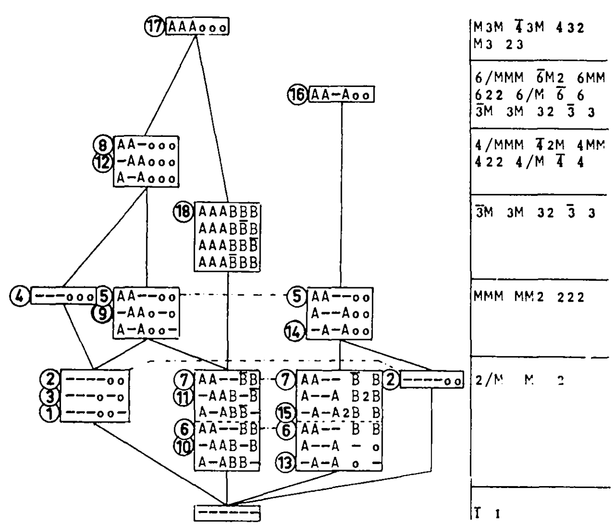

Fig. 1. Symmetry-imposed β-restrictions for all special positions.

The anisotropic atomic temperature factor may be defined as $\exp\,[-(\sum_{i=1}^{3}\sum_{j=1}^{3} h_ih_j\beta_{ij})]$. The β_{ij} are the 9 contravariant components of a symmetric second-order tensor (Levy, 1956), while h_i is the ith index of a reflexion hkl. Terms with $i\neq j$ may be combined two by two: $h_ih_j\beta_{ij}+h_jh_i\beta_{ji}=2h_ih_j\beta_{ij}$,

Table 1. *The 18 β-restrictions that occur when only the first atom of an equivalent set given by Vol.* I *of* International Tables *is considered*

I	B11	B22	B33	2B12	2B23	2B13
1				o	o	
2					o	o
3				o		o
4				o	o	o
5	A	A			o	o
6	A	A			B	B
7	A	A			−B	B
8	A	A		o	o	o
9		A	A	o		o
10		A	A	B		B
11		A	A	−B		B
12		A	A	o	o	o
13		A		A	o	
14		A		A	o	o
15		A		A	2B	B
16	A	A		A	o	o
17	A	A	A	o	o	o
18	A	A	A	B	B	B

Table 2. *Nature of the β-restrictions for all space groups and for every special position indicated by means of Table* 1

SPGR	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1															
2															
3	2	2	2	2											
3	1	1	1	1											
4															
4															
5	2	2													
5	1	1													
6	2	2													
6	1	1													
7															
7															
8	2														
8	1														
9															
9															
10	2	2	2	2	2	2	2	2	2	2	2	2	2	2	
10	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
11					2										
11					1										
12	2	2	2	2			2	2	2						
12	1	1	1	1			1	1	1						
13					2	2									
13					1	1									
14															
14															
15					2										
15					1										
16	4	4	4	4	4	4	4	4	3	3	3	3	1	1	1
	P	Q	R	S	T										
	1	2	2	2	2										
17	3	3	1	1											
18	2	2													
19															
20	3	1													
21	4	4	4	4	3	3	1	1	2	2	2				
22	4	4	4	4	3	1	2	2	1	3					
23	4	4	4	4	3	3	1	1	2	2					
24	3	1	2												
25	4	4	4	4	1	1	3	3							
26	3	3													
27	2	2	2	2											
28	2	2	3												
29															
30	2	2													
31	3														
32	2	2													
33															
34	2	2													
35	4	4	2	1	3										
36	3														
37	2	2	2												
38	4	4	1	3	3										
39	2	2	1												
40	2	3													
41	2														
42	4	2	3	1											
43	2														
44	4	4	1	3											
45	2	2													
46	2	3													
47	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
	P	Q	R	S	T	U	V	W	X	Y	Z				
	4	4	4	4	4	3	3	1	1	2	2				
48	4	4	4	4			3	3	1	1	2	2			
49	2	2	2	2	4	4	4	4	3	3	1	1	2	2	2
	P	Q													
	2	2													
50	4	4	4	4			3	3	1	1	2	2			
51	1	1	1	1	4	4	1	1	1	1	3				
52			2	3											
53	3	3	3	3	3	3	1	3							
54			1	2	2										
55	2	2	2	2	2	2	2	2							
56			2	2											
57			3	2											
58	2	2	2	2	2	2	2								
59	4	4			3	1									
60			1												
61															
62			1												
63	3	3	4		3	3	2								
64	3	3		3	1	3									
65	4	4	4	4	2	2	4	4	4	4	4	4	2	3	1
	P	Q													
	2	2													
66	4	4	2	2	2	2	3	1	2	2	2	2			
67	4	4	3	3	1	1	4	3	3	1	1	2	3	1	
68	4	4			3	1	2	2							
69	4	4	3	1	2	4	4	4	4	2	1	3	3	1	2
70	4	4			3	1	2								
71	4	4	4	4	4	4	4	4	4	4		3	1	2	
72	4	4	2	2		3	1	2	2	2					
73			3	1	2										
74	3	3	1	1	4	3	1	3	1						
75	8	8	2												
76															
77	2	2	2												
78															
79	8	2													
80	2														
81	8	8	8	8	2	2	2								
82	8	8	8	8	2	2									
83	8	8	8	8	2	2	8	8	2	2	2				
84	2	2	2	2	8	8	2	2	2	2					
85	8	8	8			2									
86	8	8			2	2									
87	8	8	2	8	8		2	2							
88	8	8			2										
89	8	8	8	8	4	4	8	8	2	7	7	3	3	3	3
90	5	5	8	2	7	7									

SPGR	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
91	1	1	7												
92	7														
93	4	4	4	4	5	5	2	2	2	3	3	3	3	7	7
94	5	5	2	2	7	7									
95	1	1	7												
96	7														
97	8	8	4	5	8	2	7	3	3	7					
98	5	5	2	7	6	3									
99	8	8	4	6	1	1									
100	8	5	6												
101	5	5	2	6											
102	5	2	6												
103	8	8	2												
104	8	2													
105	4	4	4	1	1										
106	2	2													
107	8	4	6	1											
108	8	5	6												
109	4	3													
110	2														
111	8	8	8	8	4	4	5	5	3	3	3	3	2	6	
112	4	4	4	4	8	8	3	1	3	1	2	2	2		
113	8	8	5	2	6										
114	8	8	2	2											
115	8	8	8	8	4	4	4	7	7	1	1				
116	5	5	8	8	7	7	2	2	2						
117	8	8	5	5	2	2	7	7							
118	8	8	5	5	2	6	7	2							
119	8	8	8	8	4	4	7	7	1						
120	5	8	8	5	7	2	2	7							
121	8	8	4	8	5	3	3	2	6						
122	8	8	2	3											
123	8	8	8	8	4	4	8	8	4	5	5	4	4	4	4
	P	Q	R	S	T										
	2	2	6	1	1										
124	8	8	8	8	2	4	8	8	2	7	3	3	2		
125	8	8	8	8	7	7	8	5	7	7	3	3	7		
126	8	8	4	8	8		2	7	3	3					
127	8	8	5	5	8	5	5	5	2	2	6				
128	8	8	2	5	8	2	7	2							
129	8	8	8	6	6	4	6	6	3	6					
130	5	8	8		2	6									
131	4	4	4	4	8	8	4	4	4	4	4	4	4	7	3
	P	Q													
	3	2													
132	5	8	5	8	4	2	5	5	5	5	2	3	3	2	6
133	4	4	5	8		2	2	3	3	7					
134	8	8	4	5	7	7	5	2	3	3	7	7	7		
135	2	8	2	5	2	2	7	2							
136	5	5	2	8	5	5	5	2	2	6					
137	8	8	4	4		6	3								
138	5	8	6	6	5	2	6	6	6						
139	8	8	4	8	8	6	4	5	4	4	7	2	6	3	
140	8	8	8	5	7	8	5	5	7	3	2	6			
141	8	8	3	3	4	3	7	3							
142	8	5		2	3	7									
143	16	16	16												
144															
145															
146	18														
146	16														
147	16	16	16	16											
148	18	18	18												
148	16	16	16												
149	16	16	16	16	16	16	16	16	16	6	6				
150	16	16	16	16	15	15									
151	6	6													
152	15	15													
153	6	6													
154	15	15													
155	18	18	18	10	10										
155	16	16	16	15	15										
156	16	16	16	7											
157	16	16	13												
158	16	16	16												
159	16	16													
160	18	6													
160	16	7													
161	18														
161	16														
162	16	16	16	16	16	13	13	16	6	6	13				
163	16	16	16	16	16	16		6							
164	16	16	16	16	15	15	15	15	7						
165	16	16	16	16		15									
166	18	18	18	10	10	6	6	6							
166	16	16	16	15	15	15	15	7							
167	18	18	18		6										
167	16	16	16		15										
168	16	16	2												
169															
170															
171	2	2													
172	2	2													
173	16	16													
174	16	16	16	16	16	16	16	16	16	2	2				
175	16	16	16	16	16	2	2	16	2	2	2				
176	16	16	16	16	16	16		2							
177	16	16	16	16	16	14	14	16	2	15	15	6	6		
178	15	13													
179	15	13													
180	14	14	14	14	2	2	15	15	13	13					
181	14	14	14	14	2	2	15	15	13	13					
182	16	16	16	16	16	16	15	13							
183	16	16	14	13	7										
184	16	16	2												
185	16	16	13												
186	16	16	7												
187	16	16	16	16	16	16	16	16	16	5	5	2	2	7	
188	16	16	16	16	16	16	16	16	16	6	2				
189	16	16	16	16	16	14	14	16	13	2	2				
190	16	16	16	16	16	16	15	2							

Table 2 (*cont.*)

SPGR	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
191	16	16	16	16	16	14	14	16	14	14	14	14	14	13	15
	P	Q													
	2	2													
192	16	16	16	16	16	14	2	16	2	15	13	2			
193	16	16	16	16	16	13	14	16	13	2	13				
194	16	16	16	16	16	16	15	14	15	2	15				
195	17	17	4	4	18	3	3	3	3						
196	17	17	17	17	18	3	3								
197	17	4	18	3	3										
198	18														
199	18	3													
200	17	17	4	4	4	4	4	4	18	3	3				
201	17	18	18	4	18	3	3								
202	17	17	17	3	4	18	3	3							
203	17	17	18	18	18	3									
204	17	4	18	4	4	18	3								
205	18	18	18												
206	18	18	18	3											
207	17	17	12	12	12	12	18	3	11	11					
208	17	18	18	4	9	9	18	3	3	3	10	11			
209	17	17	17	9	12	18	11	11	3						

SPGR	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
210	17	17	18	18	18	3	10								
211	17	12	18	9	12	18	3	11	10						
212	18	18	18	10											
213	18	18	18	11											
214	18	18	9	9	18	3	11	10							
215	17	17	12	12	18	9	9	3	6						
216	17	17	17	17	18	9	9	6							
217	17	12	18	12	9	3	6								
218	17	4	12	12	18	3	3	3							
219	17	17	12	12	18	3	3								
220	12	12	18	3											
221	17	17	12	12	12	12	18	4	9	9	3	3	6		
222	17	12	18	12	12	18	3	11							
223	17	4	12	12	18	4	4	4	18	11	3				
224	17	18	18	12	18	9	9	3	10	11	6				
225	17	17	17	9	12	18	9	9	9	3	6				
226	17	17	12	12	4	12	18	11	3						
227	17	17	18	18	18	9	6	10							
228	17	18	18	12	18	3	10								
229	17	12	18	12	12	18	4	9	10	3	6				
230	18	18	9	12	18	3	10								

reducing the number of terms in the exponent from 9 to 6 and introducing the explicit factor 2.

For an anisotropic atom in a special position both position and (if the point symmetry is higher than $\bar{1}$) orientation of the ellipsoidal atomic charge distribution are constrained by symmetry, resulting in a decrease of the number of independent parameters from 3 to either 2, 1 or 0 for its position and from 6 to either 4, 3, 2 or 1 for its vibration tensor. It is well known that the decreased number of independent variables may lead to singular matrices in the least-squares normal equations, and to erroneous parameter shifts, if no special measures are taken.

In order to determine the extent of such measures the present paper states the number and nature of the symmetry-imposed restrictions on the values of the β_{ij} for all special positions (Fig. 1). We will refer to such restrictions as β-restrictions. In addition we have produced Tables 1 and 2, which allow a rapid identification of the β-restrictions for any special position in the 230 space groups, analogous to the coordinate information of *International Tables for X-ray Crystallography* (1952).

β-Restrictions occur only when an atomic position is invariant to the operation of one or more proper or improper rotation axes (barring $\bar{1}$). An investigation of the number and nature of the β-restrictions therefore reduces to a point symmetry problem, and it suffices to study only $m3m$ and $6/mmm$, of which all other point groups are subgroups.

Furthermore, a representation of atomic vibration by the second-order tensor β implies that the atomic symmetry is one of the following:

(*a*) A sphere (symmetry $\infty\infty\infty$) in positions of symmetry 23 and its supergroups,

(*b*) An ellipsoid of revolution (symmetry ∞/m) in positions of symmetry 3, 4, $\bar{4}$ and 'non-cubic' supergroups,

(*c*) A general ellipsoid. In special positions with point symmetry 222 or its 'orthorhombic' supergroups the orientation of all three principal axes of vibration with respect to the crystallographic axes will be fixed by symmetry; in positions of symmetry 2 (or m) or its supergroup $2/m$ the orientation of only one principal vibration axis is fixed by point symmetry.

It follows from these considerations that the number of β-restrictions is the number of orientations with respect to the crystallographic axes in which the groups of symmetry elements 23, 4, 3, 222 and 2 are present as subgroups in the point groups $m3m$ and $6/mmm$. ($\bar{4}$ need not be investigated, as its orientation with reference to the axes is obviously the same as that of 4 in all cases; an analogous situation exists with respect to m: all β-restrictions caused by a mirror plane also occur as a result of a twofold axis perpendicular to the plane, which is always present as subgroup in the required orientation in both $m3m$ and $6/mmm$). Reasoning along these lines 28 cases of β-restrictions are found to exist. They are displayed in Fig. 1. The six symbols on one line in the boxes represent β_{11}, β_{22}, β_{33}, $2\beta_{12}$, $2\beta_{23}$, $2\beta_{13}$, respectively. A dash indicates an unrestricted component; identical components are represented by symbols A or B occurring more than once on the same line, *etc.* All symmetry-equivalent cases of β-restrictions are grouped in one box, the symmetry of the special position in question being stated at the right side of Fig. 1. The solid lines connecting the boxes indicate how, when starting with a spherical atom in a position of symmetry $m3m$ (top left) and an ellipsoid of revolution of symmetry $6/mmm$ (top right), all other cases of β-restrictions can be produced by a relaxation of symmetry demands. Identical β-restrictions occurring twice in this process are connected by chain-dotted lines. The numbers preceding the boxes refer to Tables 1 and 2.

Table 1 contains the 18 cases of β-restrictions that occur when only the first atom given by Vol. I of *International Tables* for a certain special position is considered. Table 2 presents, for all space groups (top to bottom in a column), and for every special position (left to right) of point symmetry higher than $\bar{1}$ an integer, which, by means of Table 1, indicates the nature of the β-restriction for the first atom of the equivalent set. All monoclinic space groups are entered twice: the first entry refers to the first setting (c axis unique); the second to the setting with the b axis as the unique axis. Similarly rhombohedral space groups occur twice: first with a rhombohedral unit cell, then with the alternative choice of hexagonal axes. Tetragonal and cubic space groups have all been processed with such a choice of unit cell as to have the origin on a centre of symmetry.

The (electronic) computation of this table proceeded as follows:

Space group information consisting of the multiplicity (M) and the coded coordinates of the equivalent general positions were fed into the machine. All symmetry-equivalent positions $\mathbf{x}_s$ were generated by the operation of a 3×3 rotation matrix R on a position $\mathbf{x}$, followed by the addition of a translation vector $\mathbf{t}_s$:

$$\mathbf{x}_s = R_s\mathbf{x} + \mathbf{t}_s \qquad (1)$$

(*cf.* Cruickshank, 1961), and subsequently all (M) matrices R_s and vectors $\mathbf{t}_s$ were assembled. Next all R_s and $\mathbf{t}_s$ operated upon the coordinates of the first atom of a special position of multiplicity m. Naturally, of the M general positions thus generated, M/m coincided with the first atom, and in this way the M/m transformations that left the special position invariant could be identified.

Now the β_{ij} (constituting a second-order tensor) transform as follows:

$$\beta'_{ij} = \sum_{k=1}^{3} \sum_{l=1}^{3} R_{ik} R_{jl} \beta_{kl} \, , \tag{2}$$

the matrices R being identical with those in (1). An arbitrary symmetric tensor β was subsequently subjected to the M/m transformations (2), employing the M/m matrices R that left the atomic position invariant. The invariant tensor β_{inv} that displays the desired β-restrictions was then constructed by an application of Wigner's theorem (Wigner, 1931):

$$(\beta_{\mathrm{inv}})_{ij} = \sum_{s=1}^{M/m} (\beta'_s)_{ij} \, , \tag{3}$$

stating that the invariant tensor can be obtained by a simple summation over the corresponding elements of the symmetry-equivalent, arbitrary tensors of the coinciding atoms*. Finally the nature of the invariant tensor was analyzed by a comparison with the 18 tensors of Table 1, a built-in check insuring that no other cases presented themselves.

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* A trivial application of Wigner's theorem is the derivation of coordinates of special positions (first-order tensor components) by a summation over the coordinates of certain general positions.

Acta Cryst. (1966). **20**, 150

Triple fault in face-centred cubic crystals.

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(*Received* 16 *April* 1965 *and in revised form* 17 *July* 1965)

The face-centred cubic structure [Fig. 1(*a*)] may contain various types of faults in stacking of the close-packed atomic layers (111). In Fig. 1(*b*), (*c*), and (*d*) three examples of such stacking faults are illustrated: the 'single (or intrinsic) fault', the 'double (or extrinsic) fault', and the 'triple fault'. The diffraction theories of the first two were given by Paterson (1952) and by Johnson (1963) and Warren (1963), respectively. The last one is dealt with in the present paper.

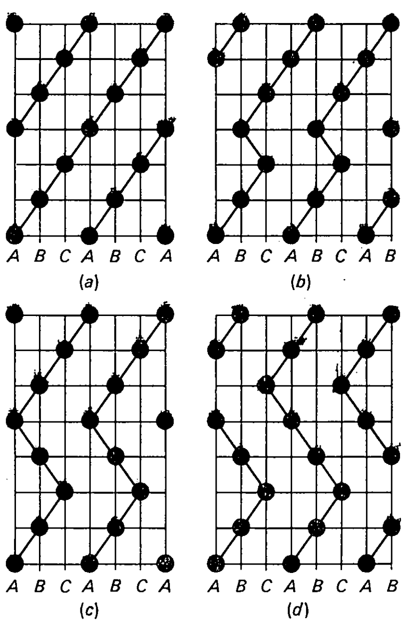

Fig. 1. (*a*) The unit-layer stacking in the face-centred cubic structure. (*b*), (*c*), and (*d*) contain a single fault, a double fault, and a triple fault, respectively. The horizontal lines are the sections of the unit-layers.

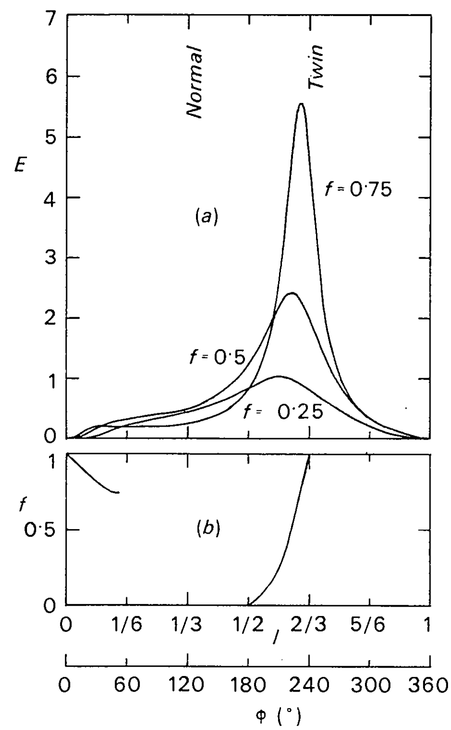

Fig. 2. (*a*) The function E for $h-k=1$ mod 3 for various values of f. The curves for $h-k=-1$ mod 3 are obtained by replacing l by $-l$. (*b*) Change in peak position of E in (*a*) as a function of f. $\varphi = 360° \times l$.