Table 4.1 *The eighteen β_{ij} restrictions for the first atom of an equivalent set given in Volume* 1 *of International Tables* (After Peterse and Palm 1966)

Case number	β_{11}	β_{22}	β_{33}	$2\beta_{12}$	$2\beta_{13}$	$2\beta_{23}$
1				0		0
2					0	0
3				0	0	
4				0	0	0
5	*A*	*A*			0	0
6	*A*	*A*			*B*	*B*
7	*A*	*A*			*B*	$-B$
8	*A*	*A*		0	0	0
9		*A*	*A*	0	0	
10		*A*	*A*	*B*	*B*	
11		*A*	*A*	$-B$	*B*	
12		*A*	*A*	0	0	0
13		*A*		*A*		0
14		*A*		*A*	0	0
15		*A*		*A*	*B*	$2B$
16	*A*	*A*		*A*	0	0
17	*A*	*A*	*A*	0	0	0
18	*A*	*A*	*A*	*B*	*B*	*B*

Peterse and Palm have compiled a second table, table 4.2, which is used in conjunction with table 4.1 to yield the β_{ij} restrictions for all the special positions listed in the *International Tables of X-ray Crystallography*, Volume 1 (1952). The columns in table 4.2 refer to the 230 space groups, and the rows to the symbols *a*, *b*, *c*, ... used in the *International Tables* to denote special positions of any space group. All monoclinic space groups are entered twice: the first entry is for a unique *c*-axis, and the second entry for a unique *b*-axis. Rhombohedral space groups also occur twice: first with a rhombohedral unit cell and then with the alternative choice of a hexagonal cell. For the tetragonal and cubic space groups the centre of symmetry, if present, coincides with the origin of the unit cell. The nature of the β_{ij} restrictions for the *first* atomic coordinates in an equivalent set in the *International Tables* is given by the appropriate numerical index in table 4.2 which refers to one of the eighteen cases listed in table 4.1.

For each space group the *International Tables* give the symmetry restrictions on the fractional coordinates *xyz* of all atoms in special positions. If used in conjunction with tables 4.1 and 4.2 of Peterse and Palm, the *International Tables* also give the symmetry restrictions on the β_{ij} coefficients. This information is required for many structure-factor refinement programs.

Peterse and Palm consider only the *first* atom of each equivalent set of special positions listed under each space group of the *International Tables*.

Table 4.2 (*cont.*)

Space group	Special position													
	a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*	*m*	*n*	*o*
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															

Table 4.2 *The β_{ij} restrictions for all space groups and for every special position: to be used in conjunction with table* 4.1 (After Peterse and Palm 1966)

Space group	Special position													
	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													

Table 4.2 (*cont.*)

Space group	Special position													
	a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*	*m*	*n*	*o*
77	2	2	2												
78															
79	8	2													
80															
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									
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		

Table 4.2 (cont.)

Space group	Special position													
	a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*	*m*	*n*	*o*
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							

Table 4.2 (cont.)

Space group	Special position													
	a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*	*m*	*n*	*o*
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		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	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							
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						
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											

Table 4.2 (cont.)

Space group	Special position													
	a	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*	*l*	*m*	*n*	*o*
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	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								

In using most refinement programs, it is sufficient to know the β_{ij} restrictions for one atom only of a symmetry-related set. This is because symmetry operations in the program are usually applied to the Miller indices rather than to the atomic coordinates. The determination of the symmetry relations among the β_{ij}s of a symmetry-related set are discussed by Trueblood (1956) and in the book of Lipson and Cochran (1966). They are derived in the same way as the symmetry restrictions for an individual member of the set.

4.4.6. *An example: sodium nitrate*

To illustrate the concept of the ellipsoid of thermal vibration, we refer to some recent neutron diffraction measurements on a crystal of sodium nitrate (Paul and Pryor 1972).

The structure of sodium nitrate, which is closely related to the cubic rock-salt structure, may be envisaged as follows. Suppose the cubic cell of NaCl, set up with a three-fold axis vertical, is compressed along this axis until the edges make an angle of 102° 42′ with each other, to give a face-centred rhombohedral cell. Each chlorine atom is then replaced by a nitrate group consisting of a central nitrogen atom with three oxygen atoms around it at the corners of an equilateral triangle. The three oxygens are 2.11 Å apart, and the whole group lies in a plane at right angles to the three-fold axis. The rhombohedral cell contains four $NaNO_3$ units, corresponding to the four NaCl units in the rock-salt structure.

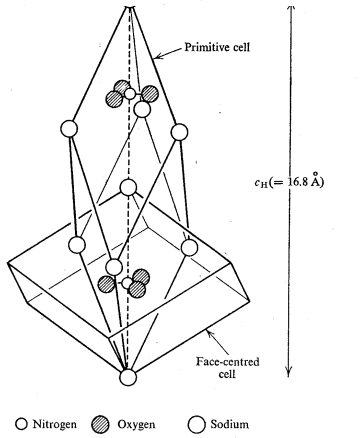

Fig. 4.5. Structure of sodium nitrate showing primitive rhombohedral cell and face-centred rhombohedral cell. Three-fold axis shown as broken line.

However, this is not the primitive rhombohedral cell. The primitive cell (figure 4.5) contains two $NaNO_3$ units, with sodium ions at the corners and centre of the cell and two nitrate groups, inversely related to each other, on the central three-fold axis. Table 4.3 gives the cell edge and rhombohedral angle for this primitive unit cell (denoted a_R and α_R respectively) and for the face-centred cell (denoted a'_R and α'_R). a_H and c_H in table 4.3 refer to the dimensions of the hexagonal cell which corresponds to the primitive rhombohedral cell. The atomic positions in $NaNO_3$ are special positions in the space group *R3c* (number 167 of *International Tables*), and are described in the Tables in terms of either the primitive rhombohedral cell (first setting) or the corresponding hexagonal cell (second setting).