

## 2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.12. Dynamical extinction lines appearing in HOLZ reflections for crystal space groups that have mirror and glide planes

 Point groups  $m$ ,  $2/m$  (second setting, unique axis  $b$ )

Space group	Incident-beam direction	
	[ $u0w$ ]	
6 $Pm$		
7 $Pc$	$h0l_0$ $c$	$A_h$
8 $Cm$		
9 $Cc$	$h_e0l_0$ $c$	$A_h$
10 $P2/m$		
11 $P2_1/m$		
12 $C2/m$		
13 $P2/c$	$h0l_0$ $c$	$A_h$
14 $P2_1/c$	$h0l_0$ $c$	$A_h$
15 $C2/c$	$h_e0l_0$ $c$	$A_h$

 Point group  $mm2$ 

Space group	Incident-beam direction									
	[100]		[010]		[001]		[0vw]		[ $u0w$ ]	
25 $Pmm2$										
26 $Pmc2_1$	$h0l_0$ $c$	$A$			$h0l_0$ $c$	$A$			$h0l_0$ $c$	$A_h$
27 $Pcc2$	$h0l_0$ $c_2$	$A$	$0kl_0$ $c_1$	$A$	$0kl_0$ $c_1$ $h0l_0$ $c_2$	$A$	$0kl_0$ $c_1$	$A_h$	$h0l_0$ $c_2$	$A_h$
28 $Pma2$	$h_00l$ $a$	$A$			$h_00l$ $a$	$A$			$h_00l$ $a$	$A_h$
29 $Pca2_1$	$h_00l$ $a$	$A$	$0kl_0$ $c$	$A$	$0kl_0$ $c$ $h_00l$ $a$	$A$	$0kl_0$ $c$	$A_h$	$h_00l$ $a$	$A_h$
30 $Pnc2$	$h0l_0$ $c$	$A$	$0kl$ : $k + l = 2n + 1$ $n$	$A$	$0kl$ : $k + l = 2n + 1$ $n$ $h0l_0$ $c$	$A$	$0kl$ : $k + l = 2n + 1$ $n$	$A_h$	$h0l_0$ $c$	$A_h$
31 $Pmn2_1$	$h0l$ : $h + l = 2n + 1$ $n$	$A$			$h0l$ : $h + l = 2n + 1$ $n$	$A$			$h0l$ : $h + l = 2n + 1$ $n$	$A_h$
32 $Pba2$	$h_00l$ $a$	$A$	$0k_0l$ $b$	$A$	$0k_0l$ $b$ $h_00l$ $a$	$A$	$0k_0l$ $b$	$A_h$	$h_00l$ $a$	$A_h$
33 $Pna2_1$	$h_00l$ $a$	$A$	$0kl$ : $k + l = 2n + 1$ $n$	$A$	$0kl$ : $k + l = 2n + 1$ $n$ $h_00l$ $a$	$A$	$0kl$ : $k + l = 2n + 1$ $n$	$A_h$	$h_00l$ $a$	$A_h$
34 $Pnn2$	$h0l$ : $h + l = 2n + 1$ $n_2$	$A$	$0kl$ : $k + l = 2n + 1$ $n_1$	$A$	$0kl$ : $k + l = 2n + 1$ $n_1$ $h0l$ : $h + l = 2n + 1$ $n_2$	$A$	$0kl$ : $k + l = 2n + 1$ $n_1$	$A_h$	$h0l$ : $h + l = 2n + 1$ $n_2$	$A_h$
35 $Cmm2$ $ba2$										
36 $Cmc2_1$ $bn2_1$	$h_e0l_0$ $c$	$A$			$h_e0l_0$ $c$	$A$			$h_e0l_0$ $c$	$A_h$
37 $Ccc2$ $nn2$	$h_e0l_0$ $c_2$	$A$	$0k_e l_0$ $c_1$	$A$	$0k_e l_0$ $c_1$ $h_e0l_0$ $c_2$	$A$	$0k_e l_0$ $c_1$	$A_h$	$h_e0l_0$ $c_2$	$A_h$

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

Space group	Incident-beam direction										
	[100]		[010]		[001]		[0vw]		[u0w]		
38 <i>Amm2</i> <i>nc2<sub>1</sub></i>											
39 <i>Abm2</i> <i>cc2<sub>1</sub></i>			$0k_o l_o$ <i>b</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A_h</i>			
40 <i>Ama2</i> <i>nn2<sub>1</sub></i>	$h_o 0l_e$ <i>a</i>	<i>A</i>			$h_o 0l_e$ <i>a</i>	<i>A</i>			$h_o 0l_e$ <i>a</i>	<i>A_h</i>	
41 <i>Aba2</i> <i>cn2<sub>1</sub></i>	$h_o 0l_e$ <i>a</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A</i>	$0k_o l_o$ <i>b</i> $h_o 0l_e$ <i>a</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A_h</i>	$h_o 0l_e$ <i>a</i>	<i>A_h</i>	
42 <i>Fmm2</i>											
43 <i>Fdd2</i> <i>dd2<sub>1</sub></i>	$h_e 0l_e$ : $h_e + l_e = 4n + 2$ <i>d<sub>2</sub></i>	<i>A</i>	$0k_e l_e$ : $k_e + l_e = 4n + 2$ <i>d<sub>1</sub></i>	<i>A</i>	$0k_e l_e$ : $k_e + l_e = 4n + 2$ <i>d<sub>1</sub></i> $h_e 0l_e$ : $h_e + l_e = 4n + 2$ <i>d<sub>2</sub></i>	<i>A</i>	$0k_e l_e$ : $k_e + l_e = 4n + 2$ <i>d<sub>1</sub></i>	<i>A_h</i>	$h_e 0l_e$ : $h_e + l_e = 4n + 2$ <i>d<sub>2</sub></i>	<i>A_h</i>	
44 <i>Imm2</i> <i>nm2<sub>1</sub></i>											
45 <i>Iba2</i> <i>cc2<sub>1</sub></i>	$h_o 0l_o$ <i>a</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A</i>	$0k_o l_o$ <i>b</i> $h_o 0l_o$ <i>a</i>	<i>A</i>	$0k_o l_o$ <i>b</i>	<i>A_h</i>	$h_o 0l_o$ <i>a</i>	<i>A_h</i>	
46 <i>Ima2</i> <i>nc2<sub>1</sub></i>	$h_o 0l_o$ <i>a</i>	<i>A</i>			$h_o 0l_o$ <i>a</i>	<i>A</i>			$h_o 0l_o$ <i>a</i>	<i>A_h</i>	

Point group *mmm*

Space group	Incident-beam direction											
	[100]		[010]		[001]		[uv0]		[0vw]		[u0w]	
47 <i>P2/m2/m2/m</i>												
48 <i>P2/n2/n2/n</i>	$h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i> $hk0$ : $h + k = 2n + 1$ <i>n<sub>3</sub></i>	<i>A</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i> $hk0$ : $h + k = 2n + 1$ <i>n<sub>3</sub></i>	<i>A</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i> $h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i>	<i>A</i>	$hk0$ : $h + k = 2n + 1$ <i>n<sub>3</sub></i>	<i>A_h</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i>	<i>A_h</i>	$h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i>	<i>A_h</i>
49 <i>P2/c2/c2/m</i>	$h0l_o$ <i>c<sub>2</sub></i>	<i>A</i>	$0kl_o$ <i>c<sub>1</sub></i>	<i>A</i>	$0kl_o$ <i>c<sub>1</sub></i> $h0l_o$ <i>c<sub>2</sub></i>	<i>A</i>			$0kl_o$ <i>c<sub>1</sub></i>	<i>A_h</i>	$h0l_o$ <i>c<sub>2</sub></i>	<i>A_h</i>
50 <i>P2/b2/a2/n</i>	$h_o 0l$ <i>a</i> $hk0$ : $h + k = 2n + 1$ <i>n</i>	<i>A</i>	$0k_o l$ <i>b</i> $hk0$ : $h + k = 2n + 1$ <i>n</i>	<i>A</i>	$0k_o l$ <i>b</i> $h_o 0l$ <i>a</i>	<i>A</i>	$hk0$ : $h + k = 2n + 1$ <i>n</i>	<i>A_h</i>	$0k_o l$ <i>b</i>	<i>A_h</i>	$h_o 0l$ <i>a</i>	<i>A_h</i>
51 <i>P2<sub>1</sub>/m2/m2/a</i>	$h_o k0$ <i>a</i>	<i>A</i>	$h_o k0$ <i>a</i>	<i>A</i>			$h_o k0$ <i>a</i>	<i>A_h</i>				
52 <i>P2/n2<sub>1</sub>/n2/a</i>	$h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i> $h_o k0$ <i>a</i>	<i>A</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i> $h_o k0$ <i>a</i>	<i>A</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i> $h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i>	<i>A</i>	$h_o k0$ <i>a</i>	<i>A_h</i>	$0kl$ : $k + l = 2n + 1$ <i>n<sub>1</sub></i>	<i>A_h</i>	$h0l$ : $h + l = 2n + 1$ <i>n<sub>2</sub></i>	<i>A_h</i>
53 <i>P2/m2/n2<sub>1</sub>/a</i>	$h0l$ : $h + l = 2n + 1$ <i>n</i> $h_o k0$ <i>a</i>	<i>A</i>	$h_o k0$ <i>a</i>	<i>A</i>	$h0l$ : $h + l = 2n + 1$ <i>n</i>	<i>A</i>	$h_o k0$ <i>a</i>	<i>A_h</i>			$h0l$ : $h + l = 2n + 1$ <i>n</i>	<i>A_h</i>
54 <i>P2<sub>1</sub>/c2/c2/a</i>	$h0l_o$ <i>c<sub>2</sub></i> $h_o k0$ <i>a</i>	<i>A</i>	$0kl_o$ <i>c<sub>1</sub></i> $h_o k0$ <i>a</i>	<i>A</i>	$0kl_o$ <i>c<sub>1</sub></i> $h0l_o$ <i>c<sub>2</sub></i>	<i>A</i>	$h_o k0$ <i>a</i>	<i>A_h</i>	$0kl_o$ <i>c<sub>1</sub></i>	<i>A_h</i>	$h0l_o$ <i>c<sub>2</sub></i>	<i>A_h</i>

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Table 2.5.3.12 (cont.)

Space group	Incident-beam direction											
	[100]		[010]		[001]		[uv0]		[0vw]		[u0w]	
55 $P2_1/b2_1/a2/m$	$h_00l$ $a$	A	$0k_0l$ $b$	A	$0k_0l$ $b$ $h_00l$ $a$	A			$0k_0l$ $b$	$A_h$	$h_00l$ $a$	$A_h$
56 $P2_1/c2_1/c2/n$	$h0l_0$ $c_2$ $hk0$ : $h+k=$ $2n+1$ $n$	A	$0kl_0$ $c_1$ $hk0$ : $h+k=$ $2n+1$ $n$	A	$0kl_0$ $c_1$ $h0l_0$ $c_2$	A	$hk0$ : $h+k=$ $2n+1$ $n$	$A_h$	$0kl_0$ $c_1$	$A_h$	$h0l_0$ $c_2$	$A_h$
57 $P2/b2_1/c2_1/m$	$h0l_0$ $c$	A	$0k_0l$ $b$	A	$0k_0l$ $b$ $h0l_0$ $c$	A			$0k_0l$ $b$	$A_h$	$h0l_0$ $c$	$A_h$
58 $P2_1/n2_1/n2/m$	$h0l$ : $h+l=$ $2n+1$ $n_2$	A	$0kl$ : $k+l=$ $2n+1$ $n_1$	A	$0kl$ : $k+l=$ $2n+1$ $n_1$ $h0l$ : $h+l=$ $2n+1$ $n_2$	A			$0kl$ : $k+l=$ $2n+1$ $n_1$	$A_h$	$h0l$ : $h+l=$ $2n+1$ $n_2$	$A_h$
59 $P2_1/m2_1/m2/n$	$hk0$ : $h+k=$ $2n+1$ $n$	A	$hk0$ : $h+k=$ $2n+1$ $n$	A			$hk0$ : $h+k=$ $2n+1$ $n$	$A_h$				
60 $P2_1/b2_1/c2_1/n$	$h0l_0$ $c$ $hk0$ : $h+k=$ $2n+1$ $n$	A	$0k_0l$ $b$ $hk0$ : $h+k=$ $2n+1$ $n$	A	$0k_0l$ $b$ $h0l_0$ $c$	A	$hk0$ : $h+k=$ $2n+1$ $n$	$A_h$	$0k_0l$ $b$	$A_h$	$h0l_0$ $c$	$A_h$
61 $P2_1/b2_1/c2_1/a$	$h0l_0$ $c$ $h_0k0$ $a$	A	$0k_0l$ $b$ $h_0k0$ $a$	A	$0k_0l$ $b$ $h0l_0$ $c$	A	$h_0k0$ $a$	$A_h$	$0k_0l$ $b$	$A_h$	$h0l_0$ $c$	$A_h$
62 $P2_1/n2_1/m2_1/a$	$h_0k0$ $a$	A	$0kl$ : $k+l=$ $2n+1$ $n$ $h_0k0$ $a$	A	$0kl$ : $k+l=$ $2n+1$ $n$	A	$h_0k0$ $a$	$A_h$	$0kl$ : $k+l=$ $2n+1$ $n$	$A_h$		
63 $C2/m2/c2_1/m$	$h_e0l_0$ $c$	A			$h_e0l_0$ $c$	A					$h_e0l_0$ $c$	$A_h$
64 $C2/m2/c2_1/a$	$h_e0l_0$ $c$ $h_0k_00$ $a$	A	$h_0k_00$ $a$	A	$h_e0l_0$ $c$	A	$h_0k_00$ $a$	$A_h$			$h_e0l_0$ $c$	$A_h$
65 $C2/m2/m2/m$												
66 $C2/c2/c2/m$	$h_e0l_0$ $c_2$	A	$0k_e l_0$ $c_1$	A	$0k_e l_0$ $c_1$ $h_e0l_0$ $c_2$	A			$0k_e l_0$ $c_1$	$A_h$	$h_e0l_0$ $c_2$	$A_h$
67 $C2/m2/m2/a$	$h_0k_00$ $a$	A	$h_0k_00$ $a$	A			$h_0k_00$ $a$	$A_h$				
68 $C2/c2/c2/a$	$h_e0l_0$ $c_2$ $h_0k_00$ $a$	A	$0k_e l_0$ $c_1$ $h_0k_00$ $a$	A	$0k_e l_0$ $c_1$ $h_e0l_0$ $c_2$	A	$h_0k_00$ $a$	$A_h$	$0k_e l_0$ $c_1$	$A_h$	$h_e0l_0$ $c_2$	$A_h$
69 $F2/m2/m2/m$												
70 $F2/d2/d2/d$	$h_e0l_e$ : $h_e+l_e=$ $4n+2$ $d_2$ $h_ek_e0$ : $h_e+k_e=$ $4n+2$ $d_3$	A	$h_ek_e0$ : $h_e+k_e=$ $4n+2$ $d_3$ $0k_e l_e$ : $k_e+l_e=$ $4n+2$ $d_1$	A	$0k_e l_e$ : $k_e+l_e=$ $4n+2$ $d_1$ $h_e0l_e$ : $h_e+l_e=$ $4n+2$ $d_2$	A	$h_ek_e0$ : $h_e+k_e=$ $4n+2$ $d_3$	$A_h$	$0k_e l_e$ : $k_e+l_e=$ $4n+2$ $d_1$	$A_h$	$h_e0l_e$ : $h_e+l_e=$ $4n+2$ $d_2$	$A_h$
71 $I2/m2/m2/m$												

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

Space group	Incident-beam direction											
	[100]		[010]		[001]		[uv0]		[0vw]		[u0w]	
72 $I2/b2/a2/m$	$h_00l_0$ <i>a</i>	A	$0k_0l_0$ <i>b</i>	A	$0k_0l_0$ <i>b</i> $h_00l_0$ <i>a</i>	A			$0k_0l_0$ <i>b</i>	$A_h$	$h_00l_0$ <i>a</i>	$A_h$
73 $I2_1/b2_1/c2_1/a$	$h_00l_0$ <i>c</i> $h_0k_00$ <i>a</i>	A	$h_0k_00$ <i>a</i> $0k_0l_0$ <i>b</i>	A	$0k_0l_0$ <i>b</i> $h_00l_0$ <i>c</i>	A	$h_0k_00$ <i>a</i>	$A_h$	$0k_0l_0$ <i>b</i>	$A_h$	$h_00l_0$ <i>c</i>	$A_h$
74 $I2_1/m2_1/m2_1/a$	$h_0k_00$ <i>a</i>	A	$h_0k_00$ <i>a</i>	A			$h_0k_00$ <i>a</i>	$A_h$				

Point group  $4/m$

Space group	Incident-beam direction			
	[100], [110]		[uv0]	
83 $P4/m$				
84 $P4_2/m$				
85 $P4/n$	$hk0: h + k = 2n + 1$ <i>n</i>	A	$hk0: h + k = 2n + 1$ <i>n</i>	$A_h$
86 $P4_2/n$	$hk0: h + k = 2n + 1$ <i>n</i>	A	$hk0: h + k = 2n + 1$ <i>n</i>	$A_h$
87 $I4/m$				
88 $I4_1/a$	$h_0k_00$ <i>a</i>	A	$h_0k_00$ <i>a</i>	$A_h$

Point group  $4mm$ . The symbol *a* in the column [u0w] is equivalent to the symbol *b* in the space groups of the first column.

Space group	Incident-beam direction									
	[100]		[001]		[110]		[u0w]		[uuv]	
99 $P4mm$										
100 $P4bm$	$h_00l$ <i>a</i> <sub>2</sub>	A	$0k_0l$ <i>b</i> <sub>1</sub> $h_00l$ <i>a</i> <sub>2</sub>	A			$h_00l$ <i>a</i>	$A_h$		
101 $P4_2cm$	$h0l_0$ <i>c</i> <sub>2</sub>	A	$0kl_0$ <i>c</i> <sub>1</sub> $h0l_0$ <i>c</i> <sub>2</sub>	A			$h0l_0$ <i>c</i>	$A_h$		
102 $P4_2nm$	$h0l:$ $h + l = 2n + 1$ <i>n</i> <sub>2</sub>	A	$0kl:$ $k + l = 2n + 1$ <i>n</i> <sub>1</sub> $h0l:$ $h + l = 2n + 1$ <i>n</i> <sub>2</sub>	A			$h0l:$ $h + l = 2n + 1$ <i>n</i>	$A_h$		
103 $P4cc$	$h0l_0$ <i>c</i> <sub>12</sub>	A	$0kl_0$ <i>c</i> <sub>11</sub> $h0l_0$ <i>c</i> <sub>12</sub> $hhl_0, \bar{h}hl_0$ <i>c</i> <sub>2</sub>	A	$hhl_0$ <i>c</i> <sub>2</sub>	A	$h0l_0$ <i>c</i> <sub>1</sub>	$A_h$	$hhl_0$ <i>c</i> <sub>2</sub>	$A_h$
104 $P4nc$	$h0l:$ $h + l = 2n + 1$ <i>n</i> <sub>2</sub>	A	$0kl:$ $k + l = 2n + 1$ <i>n</i> <sub>1</sub> $h0l:$ $h + l = 2n + 1$ <i>n</i> <sub>2</sub> $hhl_0, \bar{h}hl_0$ <i>c</i>	A	$hhl_0$ <i>c</i>	A	$h0l:$ $h + l = 2n + 1$ <i>n</i>	$A_h$	$hhl_0$ <i>c</i>	$A_h$
105 $P4_2mc$			$hhl_0, \bar{h}hl_0$ <i>c</i>	A	$hhl_0$ <i>c</i>	A			$hhl_0$ <i>c</i>	$A_h$
106 $P4_2bc$	$h_00l$ <i>a</i> <sub>2</sub>	A	$0k_0l$ <i>b</i> <sub>1</sub> $h_00l$ <i>a</i> <sub>2</sub> $hhl_0, \bar{h}hl_0$ <i>c</i>	A	$hhl_0$ <i>c</i>	A	$h_00l$ <i>a</i>	$A_h$	$hhl_0$ <i>c</i>	$A_h$
107 $I4mm$										

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Table 2.5.3.12 (cont.)

Space group	Incident-beam direction									
	[100]		[001]		[110]		[u0w]		[uuv]	
108 $I4cm$	$h_0l_0$ $c_2$	A	$0k_0l_0$ $c_1$ $h_00l_0$ $c_2$	A			$h_00l_0$ $c$	$A_h$		
109 $I4_1md$			$hhl_e, \bar{h}hl_e$ : $2h + l_e = 4n + 2$ $d$	A	$hhl_e$ : $2h + l_e = 4n + 2$ $d$	A			$hhl_e$ : $2h + l_e = 4n + 2$ $d$	$A_h$
110 $I4_1cd$	$h_0l_0$ $c_2$	A	$0k_0l_0$ $c_1$ $h_00l_0$ $c_2$ $hhl_e, \bar{h}hl_e$ : $2h + l_e = 4n + 2$ $d$	A	$hhl_e$ : $2h + l_e = 4n + 2$ $d$	A	$h_00l_0$ $c$	$A_h$	$hhl_e$ : $2h + l_e = 4n + 2$ $d$	$A_h$

Point group  $\bar{4}2m$ . The symbol  $a$  in the column [u0w] is equivalent to the symbol  $b$  in the space groups of the first column.

Space group	Incident-beam direction									
	[100]		[001]		[110]		[u0w]		[uuv]	
111 $P\bar{4}2m$										
112 $P\bar{4}2c$			$hhl_0, \bar{h}hl_0$ $c$	A	$hhl_0$ $c$	A			$hhl_0$ $c$	$A_h$
113 $P\bar{4}2_1m$										
114 $P\bar{4}2_1c$			$hhl_0, \bar{h}hl_0$ $c$	A	$hhl_0$ $c$	A			$hhl_0$ $c$	$A_h$
115 $P\bar{4}m2$										
116 $P\bar{4}c2$	$h0l_0$ $c_2$	A	$0kl_0$ $c_1$ $h0l_0$ $c_2$	A			$h0l_0$ $c$	$A_h$		
117 $P\bar{4}b2$	$h_00l$ $a_2$	A	$0k_0l$ $b_1$ $h_00l$ $a_2$	A			$h_00l$ $a$	$A_h$		
118 $P\bar{4}n2$	$h0l$ : $h + l = 2n + 1$ $n_2$	A	$0kl$ : $k + l = 2n + 1$ $n_1$ $h0l$ : $h + l = 2n + 1$ $n_2$	A			$h0l$ : $h + l = 2n + 1$ $n$	$A_h$		
119 $\bar{I}4m2$										
120 $\bar{I}4c2$	$h_00l_0$ $c_2$	A	$0k_0l_0$ $c_1$ $h_00l_0$ $c_2$	A			$h_00l_0$ $c$	$A_h$		
121 $\bar{I}42m$										
122 $\bar{I}42d$			$hhl_e, \bar{h}hl_e$ : $2h + l_e = 4n + 2$ $d$	A	$hhl_e$ : $2h + l_e = 4n + 2$ $d$	A			$hhl_e$ : $2h + l_e = 4n + 2$ $d$	$A_h$

Point group  $4/mmm$ . The symbol  $a$  in the column [u0w] is equivalent to the symbol  $b$  in the space groups of the first column.

Space group	Incident-beam direction										
	[100]		[001]		[110]		[u0w]		[uuv]		[uv0]
123 $P4/mmm$ $P4/m2/m2/m$											
124 $P4/mcc$ $P4/m2/c2/c$	$h0l_0$ $c_{12}$	A	$0kl_0$ $c_{11}$ $h0l_0$ $c_{12}$ $hhl_0, \bar{h}hl_0$ $c_2$	A	$hhl_0$ $c_2$	A	$h0l_0$ $c_1$	$A_h$	$hhl_0$ $c_2$	$A_h$	
125 $P4/nbm$ $P4/n2/b2/m$	$hk0$ : $h + k = 2n + 1$ $n$ $h_00l$ $a_2$	A	$0k_0l$ $b_1$ $h_00l$ $a_2$	A	$hk0$ : $h + k = 2n + 1$ $n$	A	$h_00l$ $a$	$A_h$			$hk0$ : $h + k = 2n + 1$ $n$

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

Space group	Incident-beam direction											
	[100]		[001]		[110]		[ $u0w$ ]		[ $uuv$ ]		[ $uv0$ ]	
126 $P4/nnc$ $P4/n2/n2/c$	$hk0:$ $h + k = 2n + 1$ $n_1$ $h0l:$ $h + l = 2n + 1$ $n_{22}$	A	$0kl:$ $k + l = 2n + 1$ $n_{21}$ $h0l:$ $h + l = 2n + 1$ $n_{22}$ $hhl_0, \bar{h}hl_0$ $c$	A	$hk0:$ $h + k = 2n + 1$ $n_1$ $hhl_0$ $c$	A	$h0l:$ $h + l = 2n + 1$ $n_2$	$A_h$	$hhl_0$ $c$	$A_h$	$hk0:$ $h + k = 2n + 1$ $n_1$	$A_h$
127 $P4/mbm$ $P4/m2_1/b2/m$	$h_00l$ $a_2$	A	$0k_0l$ $b_1$ $h_00l$ $a_2$	A			$h_00l$ $a$	$A_h$				
128 $P4/mnc$ $P4/m2_1/n2/c$	$h0l:$ $h + l = 2n + 1$ $n_2$	A	$0kl:$ $k + l = 2n + 1$ $n_1$ $h0l:$ $h + l = 2n + 1$ $n_2$ $hhl_0, \bar{h}hl_0$ $c$	A	$hhl_0$ $c$	A	$h0l:$ $h + l = 2n + 1$ $n$	$A_h$	$hhl_0$ $c$	$A_h$		
129 $P4/nmm$ $P4/n2_1/m2/m$	$hk0:$ $h + k = 2n + 1$ $n$	A			$hk0:$ $h + k = 2n + 1$ $n$	A					$hk0:$ $h + k = 2n + 1$ $n$	$A_h$
130 $P4/ncc$ $P4/n2_1/c2/c$	$hk0:$ $h + k = 2n + 1$ $n$ $h0l_0$ $c_{12}$	A	$0kl_0$ $c_{11}$ $h0l_0$ $c_{12}$ $hhl_0, \bar{h}hl_0$ $c_2$	A	$hk0:$ $h + k = 2n + 1$ $n$ $hhl_0$ $c_2$	A	$h0l_0$ $c_1$	$A_h$	$hhl_0$ $c_2$	$A_h$	$hk0:$ $h + k = 2n + 1$ $n$	$A_h$
131 $P4_2/mmc$ $P4_2/m2/m2/c$			$hhl_0, \bar{h}hl_0$ $c$	A	$hhl_0$ $c$	A			$hhl_0$ $c$	$A_h$		
132 $P4_2/mcm$ $P4_2/m2/c2/m$	$h0l_0$ $c_2$	A	$0kl_0$ $c_1$ $h0l_0$ $c_2$	A			$h0l_0$ $c$	$A_h$				
133 $P4_2/nbc$ $P4_2/n2/b2/c$	$hk0:$ $h + k = 2n + 1$ $n$ $h_00l$ $a_2$	A	$0k_0l$ $b_1$ $h_00l$ $a_2$ $hhl_0, \bar{h}hl_0$ $c$	A	$hk0:$ $h + k = 2n + 1$ $n$ $hhl_0$ $c$	A	$h_00l$ $a$	$A_h$	$hhl_0$ $c$	$A_h$	$hk0:$ $h + k = 2n + 1$ $n$	$A_h$
134 $P4_2/nnm$ $P4_2/n2/n2/m$	$hk0:$ $h + k = 2n + 1$ $n_1$ $h0l:$ $h + l = 2n + 1$ $n_{22}$	A	$0kl:$ $k + l = 2n + 1$ $n_{21}$ $h0l:$ $h + l = 2n + 1$ $n_{22}$	A	$hk0:$ $h + k = 2n + 1$ $n_1$	A	$h0l:$ $h + l = 2n + 1$ $n_2$	$A_h$			$hk0:$ $h + k = 2n + 1$ $n_1$	$A_h$
135 $P4_2/mbc$ $P4_2/m2_1/b2/c$	$h_00l$ $a_2$	A	$0k_0l$ $b_1$ $h_00l$ $a_2$ $hhl_0, \bar{h}hl_0$ $c$	A	$hhl_0$ $c$	A	$h_00l$ $a$	$A_h$	$hhl_0$ $c$	$A_h$		
136 $P4_2/mnm$ $P4_2/m2_1/n2/m$	$h0l:$ $h + l = 2n + 1$ $n_2$	A	$0kl:$ $k + l = 2n + 1$ $n_1$ $h0l:$ $h + l = 2n + 1$ $n_2$	A			$h0l:$ $h + l = 2n + 1$ $n$	$A_h$				

## 2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

Space group	Incident-beam direction											
	[100]		[001]		[110]		[ $u0w$ ]		[ $uw$ ]		[ $uv0$ ]	
137 $P4_2/nmc$ $P4_2/n2_1/m2/c$	$hk0$ : $h+k=$ $2n+1$ $n$	$A$	$hhl_0, \bar{h}hl_0$ $c$	$A$	$hhl_0$ $c$ $hk0$ : $h+k=$ $2n+1$ $n$	$A$			$hhl_0$ $c$	$A_h$	$hk0$ : $h+k=$ $2n+1$ $n$	$A_h$
138 $P4_2/nmc$ $P4_2/n2_1/c2/m$	$hk0$ : $h+k=$ $2n+1$ $n$ $h0l_0$ $c_2$	$A$	$0kl_0$ $c_1$ $h0l_0$ $c_2$	$A$	$hk0$ : $h+k=$ $2n+1$ $n$	$A$	$h0l_0$ $c$	$A_h$			$hk0$ : $h+k=$ $2n+1$ $n$	$A_h$
139 $I4/mmm$ $I4/m2/m2/m$												
140 $I4/mcm$ $I4/m2/c2/m$	$h_0l_0$ $c_2$	$A$	$0k_0l_0$ $c_1$ $h_0l_0$ $c_2$	$A$			$h_0l_0$ $c$	$A_h$				
141 $I4_1/amd$ $I4_1/a2m2/d$	$h_0k_00$ $a$	$A$	$hhl_c, \bar{h}hl_c$ : $2h+l_c=$ $4n+2$ $d$	$A$	$h_0k_00$ $a$ $hhl_c$ : $2h+l_c=$ $4n+2$ $d$	$A$			$hhl_c$ : $2h+l_c=$ $4n+2$ $d$	$A_h$	$h_0k_00$ $a$	$A_h$
142 $I4_1/acd$ $I4_1/a2c2/d$	$h_0k_00$ $a$ $h_0l_0$ $c_2$	$A$	$0k_0l_0$ $c_1$ $h_0l_0$ $c_2$ $hhl_c, \bar{h}hl_c$ : $2h+l_c=$ $4n+2$ $d$	$A$	$h_0k_00$ $a$ $hhl_c$ : $2h+l_c=$ $4n+2$ $d$	$A$	$h_0l_0$ $c$	$A_h$	$hhl_c$ : $2h+l_c=$ $4n+2$ $d$	$A_h$	$h_0k_00$ $a$	$A_h$

 Point groups  $3m, \bar{3}m$ 

Space group	Incident-beam direction									
	[0001]		[11 $\bar{2}$ 0]		[1 $\bar{1}$ 00]		[11 $\bar{2}$ w]		[1 $\bar{1}$ 0w]	
156 $P3m1$										
157 $P31m$										
158 $P3c1$	$h\bar{h}0l_0, 0h\bar{h}l_0, \bar{h}0hl_0$ $c$	$A$			$h\bar{h}0l_0$ $c$	$A$			$h\bar{h}0l_0$ $c$	$A_h$
159 $P31c$	$hh2\bar{h}l_0, h2\bar{h}hl_0, 2\bar{h}hhl_0$ $c$	$A$	$hh2\bar{h}l_0$ $c$	$A$			$hh2\bar{h}l_0$ $c$	$A_h$		
160 $R3m$										
161 $R3c$	$h\bar{h}0l_0, 0h\bar{h}l_0, \bar{h}0hl_0$ : $h+l_0=3n$ $c$	$A_h$			$h\bar{h}0l_0$ : $h+l_0=3n$ $c$	$A_h$			$h\bar{h}0l_0$ : $h+l_0=3n$ $c$	$A_h$
162 $P\bar{3}1m$										
163 $P\bar{3}1c$	$hh2\bar{h}l_0, h2\bar{h}hl_0, 2\bar{h}hhl_0$ $c$	$A$	$hh2\bar{h}l_0$ $c$	$A$			$hh2\bar{h}l_0$ $c$	$A_h$		
164 $P\bar{3}m1$										
165 $P\bar{3}c1$	$h\bar{h}0l_0, 0h\bar{h}l_0, \bar{h}0hl_0$ $c$	$A$			$h\bar{h}0l_0$ $c$	$A$			$h\bar{h}0l_0$ $c$	$A_h$
166 $R\bar{3}m$										
167 $R\bar{3}c$	$h\bar{h}0l_0, 0h\bar{h}l_0, \bar{h}0hl_0$ : $h+l_0=3n$ $c$	$A_h$			$h\bar{h}0l_0$ : $h+l_0=3n$ $c$	$A_h$			$h\bar{h}0l_0$ : $h+l_0=3n$ $c$	$A_h$

 Point groups  $6mm, \bar{6}m2, 6/mmm$ 

Space group	Incident-beam direction									
	[0001]		[11 $\bar{2}$ 0]		[1 $\bar{1}$ 00]		[11 $\bar{2}$ w]		[1 $\bar{1}$ 0w]	
183 $P6mm$										
184 $P6cc$	$h\bar{h}0l_0, 0h\bar{h}l_0, \bar{h}0hl_0$ $c_1$ $hh2\bar{h}l_0, h2\bar{h}hl_0, 2\bar{h}hhl_0$ $c_2$	$A$	$hh2\bar{h}l_0$ $c_2$	$A$	$h\bar{h}0l_0$ $c_1$	$A$	$hh2\bar{h}l_0$ $c_2$	$A_h$	$h\bar{h}0l_0$ $c_1$	$A_h$

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

Space group	Incident-beam direction										
	[0001]			[11 $\bar{2}$ 0]		[1 $\bar{1}$ 00]		[11 $\bar{2}$ w]		[1 $\bar{1}$ 0w]	
185 $P6_3cm$	$h\bar{h}0l_o, 0h\bar{h}l_o, \bar{h}0hl_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A_h</i>	
186 $P6_3mc$	$hh\bar{2}hl_o, h\bar{2}hhl_o, \bar{2}hhl_o$ <i>c</i>	<i>A</i>	$hh\bar{2}hl_o$ <i>c</i>	<i>A</i>			$hh\bar{2}hl_o$ <i>c</i>	<i>A_h</i>			
187 $P\bar{6}m2$											
188 $P\bar{6}c2$	$h\bar{h}0l_o, 0h\bar{h}l_o, \bar{h}0hl_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A_h</i>	
189 $P\bar{6}2m$											
190 $P\bar{6}2c$	$hh\bar{2}hl_o, h\bar{2}hhl_o, \bar{2}hhl_o$ <i>c</i>	<i>A</i>	$hh\bar{2}hl_o$ <i>c</i>	<i>A</i>			$hh\bar{2}hl_o$ <i>c</i>	<i>A_h</i>			
191 $P6/mmm$											
192 $P6/mcc$	$h\bar{h}0l_o, 0h\bar{h}l_o, \bar{h}0hl_o$ <i>c</i> <sub>1</sub> $hh\bar{2}hl_o, h\bar{2}hhl_o, \bar{2}hhl_o$ <i>c</i> <sub>2</sub>	<i>A</i>	$hh\bar{2}hl_o$ <i>c</i> <sub>2</sub>	<i>A</i>	$h\bar{h}0l_o$ <i>c</i> <sub>1</sub>	<i>A</i>	$hh\bar{2}hl_o$ <i>c</i> <sub>2</sub>	<i>A_h</i>	$h\bar{h}0l_o$ <i>c</i> <sub>1</sub>	<i>A_h</i>	
193 $P6_3/mcm$	$h\bar{h}0l_o, 0h\bar{h}l_o, \bar{h}0hl_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A</i>			$h\bar{h}0l_o$ <i>c</i>	<i>A_h</i>	
194 $P6_3/mmc$	$hh\bar{2}hl_o, h\bar{2}hhl_o, \bar{2}hhl_o$ <i>c</i>	<i>A</i>	$hh\bar{2}hl_o$ <i>c</i>	<i>A</i>			$hh\bar{2}hl_o$ <i>c</i>	<i>A_h</i>			

Point group  $m\bar{3}$

Space group	Incident-beam direction					
	[100]		[110]		[uv0]	
200 $Pm\bar{3}$ $P2_1/m\bar{3}$						
201 $Pn\bar{3}$ $P2_1/n\bar{3}$	$h0l: h + l = 2n + 1$ <i>n</i> <sub>2</sub> $hk0: h + k = 2n + 1$ <i>n</i> <sub>3</sub>	<i>A</i>	$hk0: h + k = 2n + 1$ <i>n</i> <sub>3</sub>	<i>A</i>	$hk0: h + k = 2n + 1$ <i>n</i>	<i>A_h</i>
202 $Fm\bar{3}$ $F2_1/m\bar{3}$						
203 $Fd\bar{3}$ $F2_1/d\bar{3}$	$h_e0l_e: h_e + l_e = 4n + 2$ <i>d</i> <sub>2</sub> $h_e k_e 0: h_e + k_e = 4n + 2$ <i>d</i> <sub>3</sub>	<i>A</i>	$h_e k_e 0: h_e + k_e = 4n + 2$ <i>d</i> <sub>3</sub>	<i>A</i>	$h_e k_e 0: h_e + k_e = 4n + 2$ <i>d</i>	<i>A_h</i>
204 $Im\bar{3}$ $I2_1/m\bar{3}$						
205 $Pa\bar{3}$ $P2_1/a\bar{3}$	$h0l_o$ <i>c</i> <sub>2</sub> $h_o k 0$ <i>a</i> <sub>3</sub>	<i>A</i>	$h_o k 0$ <i>a</i> <sub>3</sub>	<i>A*</i>	$h_o k 0$ <i>a</i>	<i>A_h</i>
206 $Ia\bar{3}$ $I2_1/a\bar{3}$	$h_o 0 l_o$ <i>c</i> <sub>2</sub> $h_o k_o 0$ <i>a</i> <sub>3</sub>	<i>A</i>	$h_o k_o 0$ <i>a</i> <sub>3</sub>	<i>A</i>	$h_o k_o 0$ <i>a</i>	<i>A_h</i>

Point group  $\bar{4}3m$ . The symbol *a* in the column [100] is equivalent to the symbol *c* in the space groups of the first column.

Space group	Incident-beam direction					
	[100]		[110]		[uuw]	
215 $P\bar{4}3m$						
216 $F\bar{4}3m$						
217 $I\bar{4}3m$						
218 $P\bar{4}3n$	$h_o k k, h_o \bar{k} k$ <i>n</i>	<i>A</i>	$hhl_o$ <i>n</i>	<i>A</i>	$hhl_o$ <i>n</i>	<i>A_h</i>
219 $F\bar{4}3c$	$h_o k_o k_o, h_o \bar{k}_o k_o$ <i>a</i>	<i>A</i>	$h_o h_o l_o$ <i>c</i>	<i>A</i>	$h_o h_o l_o$ <i>c</i>	<i>A_h</i>
220 $I\bar{4}3d$	$h_o k k, h_o \bar{k} k: 2k + h_e = 4n + 2$ <i>d</i>	<i>A</i>	$hhl_e: 2h + l_e = 4n + 2$ <i>d</i>	<i>A</i>	$hhl_e: 2h + l_e = 4n + 2$ <i>d</i>	<i>A_h</i>

## 2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

Table 2.5.3.12 (cont.)

 Point group  $m\bar{3}m$ . The symbol  $a$  in the column [100] is equivalent to the symbol  $c$  in the space groups of the first column.

Space group	Incident-beam direction							
	[100]		[110]		[uv0]		[uuv]	
221 $Pm\bar{3}m$ $P4/m\bar{3}2/m$								
222 $Pn\bar{3}n$ $P4/n\bar{3}2/n$	$h0l: h + l = 2n + 1$ $n_{12}$ $hk0: h + k = 2n + 1$ $n_{13}$ $h_0kk, h_0\bar{k}k$ $n_2$	A	$hk0: h + k = 2n + 1$ $n_{13}$ $hhl_0$ $n_2$	A	$hk0: h + k = 2n + 1$ $n_1$	$A_h$	$hhl_0$ $n_2$	$A_h$
223 $Pm\bar{3}n$ $P4_2/m\bar{3}2/n$	$h_0kk, h_0\bar{k}k$ $n$	A	$hhl_0$ $n$	A			$hhl_0$ $n$	$A_h$
224 $Pn\bar{3}m$ $P4_2/n\bar{3}2/m$	$h0l: h + l = 2n + 1$ $n_2$ $hk0: h + k = 2n + 1$ $n_3$	A	$hk0: h + k = 2n + 1$ $n_3$	A	$hk0: h + k = 2n + 1$ $n$	$A_h$		
225 $Fm\bar{3}m$ $F4/m\bar{3}2/m$								
226 $Fm\bar{3}c$ $F4/m\bar{3}2/c$	$h_0k_0k_0, h_0\bar{k}_0k_0$ $a$	A	$h_0h_0l_0$ $c$	A			$h_0h_0l_0$ $c$	$A_h$
227 $Fd\bar{3}m$ $F4_1/d\bar{3}2/m$	$h_0l_0c: h_e + l_e = 4n + 2$ $d_2$ $h_ek_0: h_e + k_e = 4n + 2$ $d_3$	A	$h_ek_0: h_e + k_e = 4n + 2$ $d_3$	A	$h_ek_0: h_e + k_e = 4n + 2$ $d$	$A_h$		
228 $Fd\bar{3}c$ $F4_1/d\bar{3}2/c$	$h_0l_0c: h_e + l_e = 4n + 2$ $d_2$ $h_ek_0: h_e + k_e = 4n + 2$ $d_3$ $h_0k_0k_0, h_0\bar{k}_0k_0$ $a$	A	$h_0h_0l_0$ $c$ $h_ek_0: h_e + k_e = 4n + 2$ $d_3$	A	$h_ek_0: h_e + k_e = 4n + 2$ $d$	$A_h$	$h_0h_0l_0$ $c$	$A_h$
229 $Im\bar{3}m$ $I4/m\bar{3}2/m$								
230 $Ia\bar{3}d$ $I4_1/a\bar{3}2/d$	$h_0k_00$ $a_3$ $h_0l_0$ $c_2$ $h_ek_0, h_0\bar{k}k: 2k + h_e = 4n + 2$ $d$	A	$hhl_0: 2h + l_e = 4n + 2$ $d$ $h_0k_00$ $a_3$	A	$h_0k_00$ $a$	$A_h$	$hhl_0: 2h + l_e = 4n + 2$ $d$	$A_h$

are no kinematically forbidden reflections. Thus, the lattice type is determined to be primitive  $P$ .

Possible space groups which satisfy point group  $4/m\bar{3}m$  and primitive lattice type  $P$  are those of Nos. 123–138 in Table 2.5.3.9. In Fig. 2.5.3.15(a), the dynamical extinction line  $A_2$  is seen in the 100 disc and in the equivalent 010 disc. By consulting Table 2.5.3.9, four space groups  $P4/m\bar{3}m$ ,  $P4/mnc$ ,  $P4_2/m\bar{3}c$  and  $P4_2/mnm$  are selected. In Fig. 2.5.3.15(b), the dynamical extinction line  $A_2$  is seen in the 010 disc but not in the 10 $\bar{1}$  disc. Two space groups  $P4/mnc$  and  $P4_2/mnm$  are selected from the four. To distinguish the two space groups, it is found from Table 2.5.3.9 that a CBED pattern taken with the [110] electron incidence should be examined. Fig. 2.5.3.15(e) shows a CBED pattern taken with the [110] incidence at 100 kV, where the 001 reflection is exactly excited. The  $h\bar{h}1$  reflections are kinematically allowed for space group  $P4_2/mnm$  but kinematically forbidden for  $P4/mnc$ . Since in the case of  $P4/mnc$ , no *Umweganregung* (multiple scattering) paths to the 001 reflection exist in the zeroth-order Laue zone, only the intensities of HOLZ lines, which are caused by *Umweganregung* via HOLZ reflections, are expected to appear in the 001 disc. If such *Umweganregung* is not practically excited, the 001 reflection must have no intensity. However, strong intensity produced by two-dimensional interaction is seen in the 001 disc of Fig. 2.5.3.15(e). This indicates that the reflection is an allowed reflection. Therefore, the space group of rutile is determined to be  $P4_2/mnm$ , which agrees with the space group already known.

*Samarium selenide* ( $Sm_3Se_4$ ).  $Sm_3Se_4$  has the  $Th_3P_4$  structure type with space group  $I43d$  at high temperatures. The lattice parameters are  $a = b = c = 0.8885$  nm. It was expected that  $Sm_3Se_4$  would transform to an ordered state of electrons with two valences of +2 and +3 around 150 K. The determination of the space group of the material was conducted at 100 K and room temperature. The space groups at both temperatures were determined by CBED to be the same. The following experiments were performed at 100 K.

Fig. 2.5.3.16(a) shows a CBED pattern taken with the [111] incidence at 80 kV, which clearly shows the first-order-Laue-zone reflections. The symmetry of the WP is seen to be  $3m$  with the help of the enlarged insets. Possible diffraction groups are  $3m$ ,  $3m1_R$  and  $6_Rmm_R$  from Table 2.5.3.3. Fig. 2.5.3.16(b), which is the central part of Fig. 2.5.3.16(a), shows projection symmetry  $3m$ , indicating that the projection diffraction group is  $3m1_R$ . Among the three groups  $3m$ ,  $3m1_R$  and  $6_Rmm_R$ , diffraction groups for which the projection diffraction group is  $3m1_R$  are  $3m$  and  $3m1_R$ . Possible point groups are found to be  $3m$ ,  $43m$  and  $6m2$  from Fig. 2.5.3.4. Fig. 2.5.3.16(c) shows a CBED pattern taken with the [100] incidence at 80 kV. The WP is seen to have symmetry  $2mm$ . Allowed diffraction groups are  $2mm$ ,  $2mm1_R$  and  $4_Rmm_R$ . Fig. 2.5.3.16(d), which is the central part of Fig. 2.5.3.16(c), shows projection WP symmetry  $4mm$ , indicating that the projection diffraction group is  $4mm1_R$ . The diffraction group among the three groups  $2mm$ ,  $2mm1_R$  and  $4_Rmm_R$  whose projection diffraction group is  $4mm1_R$  is  $4_Rmm_R$ . Possible point groups are found to be  $43m$  and  $42m$  from Fig. 2.5.3.4. Thus, the point group