2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions*

Point groups 2, *m*, 2/*m* (2nd setting unique axis $\parallel b$)

Space group		Incident-beam direction $[u0w]$	
4	$P2_1$	$0k0$ 2_1	S
7	Pc	$h0l$ c	G
9	Cc	$h0l$ c	G
11	$P2_1/m$	$0k0$ 2_1	S
13	$P2/c$	$h0l$ c	G
14	$P2_1/c$	$0k0$ 2_1 $- - - -$ $h0l$ c	S G
15	$C2/c$	$h0l$ c	G

Point groups 222, *mm*2

Space group		Incident-beam direction					
		$[100]$	$[010]$	$[001]$	$[uv0]$	$[0vw]$	$[u0w]$
17	$P222_1$	$00l$ 2_1 S	$00l$ 2_1 S		$00l$ 2_1 S		
18	$P2_12_12$	$0k0$ 2_1 S	$h00$ 2_1 S	$h00, 0k0$ 2_1 S		$h00$ 2_1 S	$0k0$ 2_1 S
19	$P2_12_12_1$	$0k0, 00l$ 2_1 S	$h00, 00l$ 2_1 S	$h00, 0k0$ 2_1 S	$00l$ 2_1 S	$h00$ 2_1 S	$0k0$ 2_1 S
20	$C222_1$	$00l$ 2_1 S	$00l$ 2_1 S		$00l$ 2_1 S		
26	$Pmc2_1$	$00l$ $c + 2_1$ GS	$00l$ 2_1 $c' -$		$00l$ 2_1 S		$h0l$ c G
27	$Pcc2$	$00l$ c $c' -$	$00l$ c $c' -$			$0kl$ c G	$h0l$ c G
28	$Pma2$			$h00$ a G			$h0l$ a G
29	$Pca2_1$	$00l$ 2_1 $c' -$	$00l$ $c + 2_1$ GS	$h00$ a G	$00l$ 2_1 S	$0kl$ c G	$h0l$ a G
30	$Pnc2$	$00l$ c $n' -$	$00l$ n $c' -$	$0k0$ n G		$0kl$ n G	$h0l$ c G
31	$Pmn2_1$	$00l$ $n + 2_1$ GS	$00l$ 2_1 $n' -$	$h00$ n G	$00l$ 2_1 S		$h0l$ n G
32	$Pba2$			$h00, 0k0$ a b G		$0kl$ b G	$h0l$ a G

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Space group		[100]	[010]	[001]	[uv0]	[0vw]	[u0w]
		Incident-beam direction					
33	$Pna2_1$	00l 2_1 $n'-$	00l $n+2_1$ GS	h00, 0k0 a b G	00l 2_1 S	0kl n G	h0l a G
34	$Pnn2$	00l n $n'-$	00l n $n'-$	h00, 0k0 n G		0kl n G	h0l n G
36	$Cmc2_1$	00l $c+2_1$ GS	00l 2_1 $c'-$		00l 2_1 S		h0l c G
37	$Ccc2$	00l c $c'-$	00l c $c'-$			0kl c G	h0l c G
39	$Abm2$					0kl b G	
40	$Ama2$			h00 a G			h0l a G
41	$Aba2$			h00 a G		0kl b G	h0l a G
43	$Fdd2$	00l $d'-$	00l d $d'-$	h00, 0k0 d G		0kl d G	h0l d G
45	$Iba2$	$b'-$	$a'-$			0kl b G	h0l a G
46	$Ima2$		$a'-$				h0l a G

Point group *mmm*

Space group		[100]	[010]	[001]	[uv0]	[0vw]	[u0w]
		Incident-beam direction					
48	$P\ 2/n\ 2/n\ 2/n$	00l, 0k0 n $n'-$	00l, h00 n $n'-$	0k0, h00 n $n'-$	hk0 n G	0kl n G	h0l n G
49	$P\ 2/c\ 2/c\ 2/m$	00l c $c'-$	00l c $c'-$			0kl c G	h0l c G
50	$P\ 2/b\ 2/a\ 2/n$	0k0 n $b'-$	h00 n $a'-$	0k0, h00 b a $n'-$	hk0 n G	0kl b G	h0l a G
51	$P\ 2_1/m\ 2/m\ 2/a$		h00 $a+2_1$ GS	h00 2_1 $a'-$	hk0 a G	h00 2_1 S	
52	$P\ 2/n\ 2_1/n\ 2/a$	00l, 0k0 n 2_1 $a'-$	00l, h00 n a $n'-$	0k0 $n+2_1$ GS – – – – – h00 n $n'-$	hk0 a G	0kl n G	h0l n G – – – – – 0k0 2_1 S
53	$P\ 2/m\ 2/n\ 2_1/a$	00l $n+2_1$ GS	h00, 00l a 2_1 $a'-$	h00 n $a'-$	hk0 a G – – – – – 00l 2_1 S		h0l n G

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Space group		[100]	[010]	[001]	[uv0]	[0vw]	[u0w]
				Incident-beam direction			
54	$P\,2_1/c\,2/c\,2/a$	$00l$ c $\;c'-$	$h00$ $a+2_1$ GS $\;$ — — $00l$ c $\;c'-$	$h00$ 2_1 $\;a'-$	$hk0$ a $\;G$	$0kl$ c $\;G$ ——— $h00$ 2_1 $\;S$	$h0l$ c $\;G$
55	$P\,2_1/b\,2_1/a\,2/m$	$0k0$ 2_1 $\;b'-$	$h00$ 2_1 $\;a'-$	$0k0,\,h00$ $b+2_1,\,a+2_1$ GS		$0kl$ b $\;G$ ——— $h00$ 2_1 $\;S$	$h0l$ a $\;G$ ——— $0k0$ 2_1 $\;S$
56	$P\,2_1/c\,2_1/c\,2/n$	$0k0$ $n+2_1$ GS — — $00l$ c $\;c'-$	$h00$ $n+2_1$ GS — — $00l$ c $\;c'-$	$0k0,\,h00$ 2_1 $\;n'-$	$hk0$ n $\;G$	$0kl$ c $\;G$ — — $h00$ 2_1 $\;S$	$h0l$ c $\;G$ — — $0k0$ 2_1 $\;S$
57	$P\,2/b\,2_1/c\,2_1/m$	$00l$ $c+2_1$ GS — — $0k0$ 2_1 $\;b'-$	$00l$ 2_1 $\;c'-$	$0k0$ $b+2_1$ GS	$00l$ 2_1 $\;S$	$0kl$ b $\;G$	$h0l$ c $\;G$ — — $0k0$ 2_1 $\;S$
58	$P\,2_1/n\,2_1/n\,2/m$	$00l,\,0k0$ $n\quad 2_1$ $\;n'-$	$00l,\,h00$ $n\quad 2_1$ $\;n'-$	$0k0,\,h00$ $n+2_1$ GS		$0kl$ n $\;G$ — — $h00$ 2_1 $\;S$	$h0l$ n $\;G$ — — $0k0$ 2_1 $\;S$
59	$P\,2_1/m\,2_1/m\,2/n$	$0k0$ $n+2_1$ GS	$h00$ $n+2_1$ GS	$0k0,\,h00$ 2_1 $\;n'-$	$hk0$ n $\;G$	$h00$ 2_1 $\;S$	$0k0$ 2_1 $\;S$
60	$P\,2_1/b\,2/c\,2_1/n$	$00l$ $c+2_1$ GS — — $0k0$ n $\;b'-$	$h00$ $n+2_1$ GS — — $00l$ 2_1 $\;c'-$	$0k0,\,h00$ $b\quad 2_1$ $\;n'-$	$hk0$ n $\;G$ — — $00l$ 2_1 $\;S$	$0kl$ b $\;G$ — — $h00$ 2_1 $\;S$	$h0l$ c $\;G$
61	$P\,2_1/b\,2_1/c\,2_1/a$	$00l$ $c+2_1$ GS — $0k0$ 2_1 $\;b'-$	$h00$ $a+2_1$ GS — $00l$ 2_1 $\;c'-$	$0k0$ $b+2_1$ GS — $h00$ 2_1 $\;a'-$	$hk0$ a $\;G$ $00l$ 2_1 $\;S$	$0kl$ b $\;G$ $h00$ 2_1 $\;S$	$h0l$ c $\;G$ $0k0$ 2_1 $\;S$
62	$P\,2_1/n\,2_1/m\,2_1/a$	$0k0,\,00l$ 2_1 $\;n'-$	$00l$ $n+2_1$ $h00$ $a+2_1$ GS	$0k0$ $n+2_1$ GS $h00$ 2_1 $\;a'-$	$hk0$ a $\;G$ $00l$ 2_1 $\;S$	$0kl$ n $\;G$ $h00$ 2_1 $\;S$	$0k0$ 2_1 $\;S$
63	$C\,2/m\,2/c\,2_1/m$	$00l$ $c+2_1$ GS	$00l$ 2_1 $\;c'-$		$00l$ 2_1 $\;S$		$h0l$ c $\;G$
64	$C\,2/m\,2/c\,2_1/a$	$00l$ $c+2_1$ GS	$00l$ 2_1 $\;c'-$		$hk0$ a $\;G$ ——— $00l$ 2_1 $\;S$		$h0l$ c $\;G$
66	$C\,2/c\,2/c\,2/m$	$00l$ c $\;c'-$	$00l$ c $\;c'-$			$0kl$ c $\;G$	$h0l$ c $\;G$
67	$C\,2/m\,2/m\,2/a$				$hk0$ a $\;G$		

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Space group	Incident-beam direction					
	[100]	[010]	[001]	[uv0]	[0vw]	[u0w]
68 $C\,2/c\,2/c\,2/a$	$00l$ / c $c'-$	$00l$ / c $c'-$		$hk0$ / a G	$0kl$ / c G	$h0l$ / c G
70 $F\,2/d\,2/d\,2/d$	$00l, 0k0$ / d $d'-$	$h00, 00l$ / d $d'-$	$0k0, h00$ / d $d'-$	$hk0$ / d G	$0kl$ / d G	$h0l$ / d G
72 $I\,2/b\,2/a\,2/m$	$b'-$	$a'-$			$0kl$ / b G	$h0l$ / a G
73 $I\,2/b\,2/c\,2/a$	$b'-$	$c'-$	$a'-$	$hk0$ / a G	$0kl$ / b G	$h0l$ / c G
74 $I\,2/m\,2/m\,2/a$				$hk0$ / a G		

Point groups 4, $\bar{4}$, 4/m

Space group	Incident-beam direction
	[uv0]
76 $P4_1$	$00l$ / 4_1 S
78 $P4_3$	$00l$ / 4_3 S
85 $P4/n$	$hk0$ / n G
86 $P4_2/n$	$hk0$ / n G
88 $I4_1/a$	$hk0$ / a G

Point group 422

Space group	Incident-beam direction	
	[uv0]	[0vw]
90 $P42_12$		$h00$ / 2_1 S
91 $P4_122$	$00l$ / 4_1 S	
92 $P4_12_12$	$00l$ / 4_1 S	$h00$ / 2_1 S
94 $P4_22_12$		$h00$ / 2_1 S
95 $P4_322$	$00l$ / 4_3 S	
96 $P4_32_12$	$00l$ / 4_3 S	$h00$ / 2_1 S

Point group 4mm

Space group	Incident-beam direction				
	[100]	[001]	[110]	[u0w] and [0vw]*	[uūw]
100 $P4bm$		$h00, 0k0$ / a b G		$h0l, 0kl$ / a b G	
101 $P4_2cm$	$00l$ / c $c'-$			$h0l, 0kl$ / c G	
102 $P4_2nm$	$00l$ / n $n'-$	$h00, 0k0$ / n G		$h0l, 0kl$ / n G	
103 $P4cc$	$00l$ / c $c'-$		$00l$ / c $c'-$	$h0l, 0kl$ / c G	hhl / c G
104 $P4nc$	$00l$ / n $n'-$	$h00, 0k0$ / n G	$00l$ / c $c'-$	$h0l, 0kl$ / n G	hhl / c G
105 $P4_2mc$			$00l$ / c $c'-$		hhl / c G

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Space group		[100]	[001]	[110]	$[u0w]$ and $[0vw]$*	$[u\bar{u}w]$
106	$P4_2bc$		$h00,\ 0k0$; $a\ \ b$; *G*	$00l$; c; *c'−*	$h0l,\ 0kl$; $a\ \ b$; *G*	hhl; c; *G*
108	$I4cm$				$h0l,\ 0kl$; c; *G*	
109	$I4_1md$		$hh0$, $\bar{h}h0$; d; *G*	$00l$; d; *d'−*		hhl; d; *G*
110	$I4_1cd$		$hh0$, $\bar{h}h0$; d; *G*	$00l$; d; *d'−*	$h0l,\ 0kl$; c; *G*	hhl; d; *G*

* Conditions in this column are cyclic on *h* and *k*.

Point groups $\bar{4}2m$, $4/mmm$

Space group	[100]	[001]	[110]	$[u0w]$ and $[0vw]$*	$[uuw]$	$[uv0]$
112 $P\bar{4}2c$			$00l$; c; *c'−*		hhl; c; *G*	
113 $P\bar{4}2_1m$	$0k0$; 2_1; *S*	$h00,\ 0k0$; 2_1; *S*		$0k0,\ h00$; 2_1; *S*		
114 $P\bar{4}2_1c$	$0k0$; 2_1; *S*	$h00,\ 0k0$; 2_1; *S*	$00l$; c; *c'−*	$0k0,\ h00$; 2_1; *S*	hhl; c; *G*	
116 $P\bar{4}c2$	$00l$; c; *c'−*			$h0l,\ 0kl$; c; *G*		
117 $P\bar{4}b2$		$h00,\ 0k0$; $a\ \ b$; *G*		$h0l,\ 0kl$; $a\ \ b$; *G*		
118 $P\bar{4}n2$	$00l$; n; *n'−*	$h00,\ 0k0$; n; *G*		$h0l,\ 0kl$; n; *G*		
120 $I\bar{4}c2$				$h0l,\ 0kl$; c; *G*		
122 $I\bar{4}2d$		$hh0$, $\bar{h}h0$; d; *G*	$00l$; d; *d'−*		hhl; d; *G*	
124 $P\ 4/m\ 2/c\ 2/c$	$00l$; c; *c'−*		$00l$; c; *c'−*	$h0l,\ 0kl$; c; *G*	hhl; c; *G*	
125 $P\ 4/n\ 2/b\ 2/m$	$0k0$; n; *b'−*	$h00,\ 0k0$; $a\ \ b$; *n'−*		$h0l,\ 0kl$; $a\ \ b$; *G*		$hk0$; n; *G*
126 $P\ 4/n\ 2/n\ 2/c$	$0k0$; n; $00l$; n; *n'−*	$h00,\ 0k0$; n; *n'−*	$00l$; c; *c'−*	$h0l,\ 0kl$; n; *G*	hhl; c; *G*	$hk0$; n; *G*
127 $P\ 4/m\ 2_1/b\ 2/m$	$0k0$; 2_1; *b'−*	$h00$; $a+2_1$; $0k0$; $b+2_1$; *GS*		$h0l,\ 0kl$; $a\ \ b$; *G* — — — $0k0,\ h00$; 2_1; *S*		

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Space group	[100]	[001]	[110]	[u0w] and [0vw]*	[uuw]	[uv0]
128 $P\,4/m\,2_1/n\,2/c$	$00l$, $0k0$ n 2_1 $n'-$	$h00$, $0k0$ $n+2_1$ GS	$00l$ c $c'-$	$h0l$, $0kl$ n G $0k0$, $h00$ 2_1 S	hhl c G	
129 $P\,4/n\,2_1/m\,2/m$	$0k0$ $n+2_1$ GS	$h00$, $0k0$ 2_1 $n'-$		$0k0$, $h00$ 2_1 S		$hk0$ n G
130 $P\,4/n\,2_1/c\,2/c$	$0k0$ $n+2_1$ GS - - - - $00l$ c $c'-$	$h00$, $0k0$ 2_1 $n'-$	$00l$ c $c'-$	$h0l$, $0kl$ c G - - - - $0k0$, $h00$ 2_1 S	hhl c G	$hk0$ n G
131 $P\,4_2/m\,2/m\,2/c$			$00l$ c $c-$		hhl c G	
132 $P\,4_2/m\,2/c\,2/m$	$00l$ c $c'-$			$h0l$, $0kl$ G c		
133 $P\,4_2/n\,2/b\,2/c$	$0k0$ n $b'-$	$h00$, $0k0$ a b $n'-$	$00l$ c $c'-$	$h0l$, $0kl$ G a b	hhl c G	$hk0$ n G
134 $P\,4_2/n\,2/n\,2/m$	$0k0$, $00l$ n $n'-$	$h00$, $0k0$ n $n'-$		$h0l$, $0kl$ G n		$hk0$ n G
135 $P\,4_2/m\,2_1/b\,2/c$	$0k0$ 2_1 $b'-$	$h00$, $0k0$ $a+2_1\ b+2_1$ GS	$00l$ c $c'-$	$h0l$, $0kl$ a b G - - - - $0k0$, $h00$ 2_1 S	hhl c G	
136 $P\,4_2/m\,2_1/n\,2/m$	$00l$, $0k0$ n 2 $n'-$	$h00$, $0k0$ $n+2_1$ GS		$h0l$, $0kl$ G n - - - - $0k0$, $h00$ 2_1 S		
137 $P\,4_2/n\,2_1/m\,2/c$	$0k0$ $n+2_1$ GS	$h00$, $0k0$ 2_1 $n'-$	$00l$ c $c'-$	$0k0$, $h00$ S 2_1	hhl c G	$hk0$ n G
138 $P\,4_2/n\,2_1/c\,2/m$	$0k0$ $n+2_1$ GS - - - - $00l$ c $c'-$	$h00$, $0k0$ 2_1 $n'-$		$h0l$, $0kl$ G c - - - - $0k0$, $h00$ 2_1 S		$hk0$ n G
140 $I\,4/m\,2/c\,2/m$				$h0l$, $0kl$ G c		
141 $I\,4_1/a\,2/m\,2/d$		$hh0$ $\bar{h}h0$ d $a'-$	$00l$, $\bar{h}h0$ d a $d'-$		hhl d G	$hk0$ a G
142 $I\,4_1/a\,2/c\,2/d$		$hh0$ $\bar{h}h0$ d $a'-$	$00l$, $\bar{h}h0$ d a $d'-$	$h0l$, $0kl$ c G	hhl d G	$hk0$ a G

* Conditions in this column are cyclic on h and k.

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Point groups 3m, $\bar{3}m$, 6, 6/m, 622, 6mm, $\bar{6}m$2, 6/mmm

Space group		Incident-beam direction			
		[100]	[210]	[2u u w]	[v0w]
158	$P3c1$		$000l$ / c G	$hh2\bar{h}l$ / c G	
159	$P31c$	$000l$ / c G			$h\bar{h}0l$ / c G
161	$R3c$		$000l$ / $l=6n+3$ / c G	$hh2\bar{h}l$ / c G	
163	$P\bar{3}1c$	$000l$ / c G			$h\bar{h}0l$ / c G
165	$P\bar{3}c1$		$000l$ / c G	$hh2\bar{h}l$ / c G	
167	$R\bar{3}c$		$000l$ / $l=6n+3$ / c G	$hh2\bar{h}l$ / c G	
169	$P6_1$	$000l$ / 6_1 S	$000l$ / 6_1 S		
170	$P6_5$	$00l$ / 6_5 S	$00l$ / 6_5 S		
173	$P6_3$	$000l$ / 6_3 S	$000l$ / 6_3 S		
176	$P6_3/m$	$000l$ / 6_3 S	$000l$ / 6_3 S		
178	$P6_122$	$000l$ / 6_1 S	$000l$ / 6_1 S		
179	$P6_522$	$000l$ / 6_5 S	$000l$ / 6_5 S		
182	$P6_322$	$000l$ / 6_3 S	$000l$ / 6_3 S		
184	$P6cc$	$000l$ / c $c'-$	$000l$ / c $c'-$	$hh2\bar{h}l$ / c G	$h\bar{h}0l$ / c G
185	$P6_3cm$	$000l$ / 6_3 $c'-$	$000l$ / $c+6_3$ GS	$hh2\bar{h}l$ / c G	
186	$P6_3mc$	$000l$ / $c+6_3$ GS	$000l$ / 6_3 $c'-$		$h\bar{h}0l$ / c G
188	$P\bar{6}c2$		$000l$ / c G	$hh2\bar{h}l$ / c G	
190	$P\bar{6}c2$	$000l$ / c G			$h\bar{h}0l$ / c G
192	$P6/mcc$	$000l$ / c $c'-$	$000l$ / c $c'-$	$hh2\bar{h}l$ / c G	$h\bar{h}0l$ / c G
193	$P6_3/mcm$	$00l$ / 6_3 $c'-$	$000l$ / $c+6_3$ GS	$hh2\bar{h}l$ / c G	
194	$P6_3/mmc$	$000l$ / $c+6_3$ GS	$000l$ / 6_3 $c'-$		$h\bar{h}0l$ / c G

Table 2.5.3.5. *Conditions for observation of GS bands for the 137 space groups exhibiting these extinctions* (*cont.*)

Point groups 23, *m*3, 432, *m*3*m*

Space group		Incident-beam direction			
		[100] (cyclic)	[110] (cyclic)	[uv0] (cyclic)	[uuw] (cyclic)
198	$P2_13$	00*l*, 0*k*0 2_1 — S	00*l* 2_1 — S	00*l* 2_1 — S	
201	$Pn\bar{3}$ $P2/n\bar{3}$	00*l*, 0*k*0 *n* — *n'*−		$\bar{k}h0$ *n* — G	
203	$Pd\bar{3}$ $F2/d\bar{3}$	00*l*, 0*k*0 *d* — *d'*−		$\bar{k}h0$ *d* — G	
205	$Pa\bar{3}$ $P2_1/a\bar{3}$	00*l* $c+2_1$ — GS - - - - - - 0*k*0 2_1 — *b'*−	00*l* 2_1 — S - - - - - - $\bar{h}h0$ *a* — G	00*l* 2_1 — S - - - - - - $\bar{k}h0$ *a* — G	
206	$Ia\bar{3}$ $I2_1/a\bar{3}$		$\bar{h}h0$ *a* — G	$\bar{k}h0$ *a* — G	
212	$P4_332$			00*l* 4_3 — S	
213	$P4_132$			00*l* 4_1 — S	
218	$P\bar{4}3n$		00*l* *c* — *n*−	*hhl* *c* — G	
219	$F\bar{4}3c$			*hhl* *c* — G	
220	$I\bar{4}3d$	0*kk* $0\bar{k}k$ — G *d*	00*l* — *d*− *d*	*hhl* — G *d*	
222	$Pn\bar{3}n$	00*l*, 0*k*0 *n* — *n'*−	00*l* *c* — *n*−	*hk*0 *n* — G	*hhl* *c* — G
223	$Pm\bar{3}n$		00*l* *c* — *n'*−		*hhl* *c* — G
224	$Pn\bar{3}m$	00*l*, 0*k*0 *n* — *n'*−		*hk*0 *n* — G	
226	$Fm\bar{3}c$				*hhl* *c* — G
227	$Fd\bar{3}m$	00*l*, 0*k*0 *d* — *d'*−		*hk*0 *d* — G	
228	$Fd\bar{3}c$	00*l*, 0*k*0 *d* — *d'*−		*hk*0 *d* — G	*hhl* *c* — G
230	$Ia\bar{3}d$	0*kk* $0\bar{k}k$ — *b'*− *d*	00*l*, $\bar{h}h0$ — *d'*− *d* *a*	*hk*0 — G *a*	*hhl* — G *d*

references