

1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table A1.4.3.4. Orthorhombic space groups

The expressions for A and B for the orthorhombic space groups in their standard settings [as in *IT A* (2005)] contain one, two or four terms of the form

$$pqr = p(2\pi hx)q(2\pi ky)r(2\pi lz) \tag{A1.4.3.2}$$

preceded by a signed numerical constant, where p , q and r can each be either a sine or a cosine function, and the arguments of the functions in any product of the form (A1.4.3.2) are ordered as in (A1.4.3.2). These products are given in this table as ccc , ccs , csc , scs , css and/or sss , where c and s are abbreviations for 'sin' and 'cos', respectively.

Note that pqr vanishes if at least one of p , q and r is a sine, and the corresponding index h , k or l is zero.

No.	Symbol	Origin	Parity	A	B
16	$P222$			4ccc	-4sss
17	$P222_1$		$l = 2n$	4ccc	-4sss
			$l = 2n + 1$	-4css	4scc
18	$P2_12_12$		$h + k = 2n$	4ccc	-4sss
			$h + k = 2n + 1$	-4ssc	4ccs
19	$P2_12_12_1$		$h + k = 2n; k + l = 2n$	4ccc	-4sss
			$h + k = 2n; k + l = 2n + 1$	-4css	4scc
			$h + k = 2n + 1; k + l = 2n$	-4scs	4csc
			$h + k = 2n + 1; k + l = 2n + 1$	-4ssc	4ccs
20	$C222_1$		$l = 2n$	8ccc	-8sss
			$l = 2n + 1$	-8css	8scc
21	$C222$			8ccc	-8sss
22	$F222$			16ccc	-16sss
23	$I222$			8ccc	-8sss
24	$I2_12_12_1$		h, k, l all even	8ccc	-8sss
			$h = 2n; k, l = 2n + 1$	-8scs	8csc
			$k = 2n; l, h = 2n + 1$	-8ssc	8ccs
			$l = 2n; h, k = 2n + 1$	-8css	8scc
25	$Pmm2$			4ccc	4ccs
26	$Pmc2_1$		$l = 2n$	4ccc	4ccs
			$l = 2n + 1$	-4css	4csc
27	$Pcc2$		$l = 2n$	4ccc	4ccs
			$l = 2n + 1$	-4ssc	-4sss
28	$Pma2$		$h = 2n$	4ccc	4ccs
			$h = 2n + 1$	-4ssc	-4sss
29	$Pca2_1$		$h = 2n; l = 2n$	4ccc	4ccs
			$h = 2n; l = 2n + 1$	-4scs	4scc
			$h = 2n + 1; l = 2n$	-4ssc	-4sss
			$h = 2n + 1; l = 2n + 1$	-4css	4csc
30	$Pnc2$		$k + l = 2n$	4ccc	4ccs
			$k + l = 2n + 1$	-4ssc	4sss
31	$Pmn2_1$		$h + l = 2n$	4ccc	4ccs
			$h + l = 2n + 1$	-4css	4csc
32	$Pba2$		$h + k = 2n$	4ccc	4ccs
			$h + k = 2n + 1$	-4ssc	-4sss
33	$Pna2_1$		$h + k = 2n; l = 2n$	4ccc	4ccs
			$h + k = 2n; l = 2n + 1$	-4scs	4scc
			$h + k = 2n + 1; l = 2n$	-4ssc	-4sss
			$h + k = 2n + 1; l = 2n + 1$	-4css	4csc
34	$Pnn2$		$h + k + l = 2n$	4ccc	4ccs
			$h + k + l = 2n + 1$	-4ssc	-4sss
35	$Cmm2$			8ccc	8ccs
36	$Cmc2_1$		$l = 2n$	8ccc	8ccs
			$l = 2n + 1$	-8css	8csc
37	$Ccc2$		$l = 2n$	8ccc	8ccs
			$l = 2n + 1$	-8ssc	-8sss
38	$Amm2$			8ccc	8ccs
39	$Abm2$		$k = 2n$	8ccc	8ccs
			$k = 2n + 1$	-8ssc	-8sss
40	$Ama2$		$h = 2n$	8ccc	8ccs
			$h = 2n + 1$	-8ssc	-8sss
41	$Aba2$		$h + k = 2n$	8ccc	8ccs
			$h + k = 2n + 1$	-8ssc	-8sss

1.4. SYMMETRY IN RECIPROCAL SPACE

Table A1.4.3.4 (cont.)

No.	Symbol	Origin	Parity	A	B
42	<i>Fmm2</i>			16ccc	16ccs
43	<i>Fdd2</i>		$h + k + l = 4n$	16ccc	16ccs
			$h + k + l = 4n + 1$	8(ccc - ssc - ccs - sss)	8(ccs - sss + ccc + ssc)
			$h + k + l = 4n + 2$	-16ssc	-16sss
			$h + k + l = 4n + 3$	8(ccc - ssc + ccs + sss)	8(ccs - sss - ccc - ssc)
44	<i>Imm2</i>			8ccc	8ccs
45	<i>Iba2</i>		$l = 2n$	8ccc	8ccs
			$l = 2n + 1$	-8ssc	-8sss
46	<i>Iam2</i>		$h = 2n$	8ccc	8ccs
			$h = 2n + 1$	-8ssc	-8sss
47	<i>Pmmm</i>			8ccc	0
48	<i>Pnnn</i>	(1)	$h + k + l = 2n$	8ccc	0
			$h + k + l = 2n + 1$	0	-8sss
48	<i>Pnnn</i>	(2)	$h + k = 2n; k + l = 2n$	8ccc	0
			$h + k = 2n; k + l = 2n + 1$	-8ssc	0
			$h + k = 2n + 1; k + l = 2n$	-8css	0
			$h + k = 2n + 1; k + l = 2n + 1$	-8scs	0
49	<i>Pccm</i>		$l = 2n$	8ccc	0
			$l = 2n + 1$	-8ssc	0
50	<i>Pban</i>	(1)	$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	0	-8sss
50	<i>Pban</i>	(2)	$h = 2n; k = 2n$	8ccc	0
			$h = 2n; k = 2n + 1$	-8scs	0
			$h = 2n + 1; k = 2n$	-8css	0
			$h = 2n + 1; k = 2n + 1$	-8ssc	0
51	<i>Pmma</i>		$h = 2n$	8ccc	0
			$h = 2n + 1$	-8scs	0
52	<i>Pnna</i>		$h = 2n; k + l = 2n$	8ccc	0
			$h = 2n; k + l = 2n + 1$	-8ssc	0
			$h = 2n + 1; k + l = 2n$	-8css	0
			$h = 2n + 1; k + l = 2n + 1$	-8scs	0
53	<i>Pmna</i>		$h + l = 2n$	8ccc	0
			$h + l = 2n + 1$	-8css	0
54	<i>Pcca</i>		$h = 2n; l = 2n$	8ccc	0
			$h = 2n; l = 2n + 1$	-8ssc	0
			$h = 2n + 1; l = 2n$	-8scs	0
			$h = 2n + 1; l = 2n + 1$	-8css	0
55	<i>Pbam</i>		$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	-8ssc	0
56	<i>Pccn</i>		$h + k = 2n; h + l = 2n$	8ccc	0
			$h + k = 2n; h + l = 2n + 1$	-8ssc	0
			$h + k = 2n + 1; h + l = 2n$	-8css	0
			$h + k = 2n + 1; h + l = 2n + 1$	-8scs	0
57	<i>Pbcm</i>		$k = 2n; l = 2n$	8ccc	0
			$k = 2n; l = 2n + 1$	-8css	0
			$k = 2n + 1; l = 2n$	-8ssc	0
			$k = 2n + 1; l = 2n + 1$	-8scs	0
58	<i>Pnrm</i>		$h + k + l = 2n$	8ccc	0
			$h + k + l = 2n + 1$	-8ssc	0
59	<i>Pmmn</i>	(1)	$h + k = 2n$	8ccc	0
			$h + k = 2n + 1$	0	8ccs
59	<i>Pmmn</i>	(2)	$h = 2n; k = 2n$	8ccc	0
			$h = 2n; k = 2n + 1$	-8css	0
			$h = 2n + 1; k = 2n$	-8scs	0
			$h = 2n + 1; k = 2n + 1$	-8ssc	0
60	<i>Pbcn</i>		$h + k = 2n; l = 2n$	8ccc	0
			$h + k = 2n; l = 2n + 1$	-8css	0
			$h + k = 2n + 1; l = 2n$	-8scs	0
			$h + k = 2n + 1; l = 2n + 1$	-8ssc	0
61	<i>Pbca</i>		$h + k = 2n; k + l = 2n$	8ccc	0

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Table A1.4.3.4 (cont.)

No.	Symbol	Origin	Parity	A	B
62	<i>Pnma</i>		$h + k = 2n; k + l = 2n + 1$	-8css	0
			$h + k = 2n + 1; k + l = 2n$	-8scs	0
			$h + k = 2n + 1; k + l = 2n + 1$	-8ssc	0
			$h + l = 2n; k = 2n$	8ccc	0
			$h + l = 2n; k = 2n + 1$	-8ssc	0
			$h + l = 2n + 1; k = 2n$	-8scs	0
			$h + l = 2n + 1; k = 2n + 1$	-8css	0
63	<i>Cmcm</i>		$l = 2n$	16ccc	0
			$l = 2n + 1$	-16css	0
64	<i>Cmca</i>		$k + l = 2n$	16ccc	0
			$k + l = 2n + 1$	-16css	0
65	<i>Cmmm</i>			16ccc	0
66	<i>Cccm</i>		$l = 2n$	16ccc	0
			$l = 2n + 1$	-16ssc	0
67	<i>Cmma</i>		$h = 2n$	16ccc	0
			$h = 2n + 1$	-16css	0
68	<i>Ccca</i>	(1)	$h + l = 2n$	16ccc	0
			$h + l = 2n + 1$	0	-16sss
68	<i>Ccca</i>	(2)	$k = 2n; l = 2n$	16ccc	0
			$k = 2n; l = 2n + 1$	-16ssc	0
			$k = 2n + 1; l = 2n$	-16scs	0
			$k = 2n + 1; l = 2n + 1$	-16css	0
69	<i>Fmmm</i>			32ccc	0
70	<i>Fddd</i>	(1)	$h + k + l = 4n$	32ccc	0
			$h + k + l = 4n + 1$	16(ccc - sss)	A
			$h + k + l = 4n + 2$	0	-32sss
			$h + k + l = 4n + 3$	16(ccc + sss)	-A
70	<i>Fddd</i>	(2)	$h + k = 4n; k + l = 4n; l + h = 4n$	32ccc	0
			$h + k = 4n; k + l = 4n + 2; l + h = 4n + 2$	-32ssc	0
			$h + k = 4n + 2; k + l = 4n; l + h = 4n + 2$	-32css	0
			$h + k = 4n + 2; k + l = 4n + 2; l + h = 4n$	-32scs	0
			$h + k = 4n + 2; k + l = 4n + 2;$ $l + h = 4n + 2$	-16(ccc + ssc + scs + css)	0
			$h + k = 4n + 2; k + l = 4n; l + h = 4n$	16(ccc + ssc - scs - css)	0
			$h + k = 4n; k + l = 4n + 2; l + h = 4n$	16(ccc - ssc - scs + css)	0
			$h + k = 4n; k + l = 4n; l + h = 4n + 2$	16(ccc - ssc + scs - css)	0
71	<i>Immm</i>			16ccc	0
72	<i>Ibam</i>		$l = 2n$	16ccc	0
			$l = 2n + 1$	-16ssc	0
73	<i>Ibca</i>		$h = 2n; k = 2n$	16ccc	0
			$h = 2n; k = 2n + 1$	-16scs	0
			$h = 2n + 1; k = 2n$	-16ssc	0
			$h = 2n + 1; k = 2n + 1$	-16css	0
			$k = 2n$	16ccc	0
74	<i>Imma</i>		$k = 2n$	16ccc	0
			$k = 2n + 1$	-16css	0