

Table 3-1 : Codes for Crystallographic Site Symmetry Symbols for atoms in special positions : assigned by module XDSPOS

Code	Symbol	Code	Symbol	Code	Symbol	Code	Symbol
1	1	21	422	41	3m.	61	mmm..
2	-1	22	2.22	42	3.m	62	m-3.
3	.2.	23	2mm.	43	.m	63	.-3.
4	..2	24	4mm	44	3m	64	42.2
5	2..	25	2.mm	45	-3.m	65	432
6	.m.	26	-42m	46	-3m.	66	.2.22
7	..m	27	-4m2	47	.2/m	67	.32
8	m..	28	m.2m	48	-3m	68	.3m
9	.2/m.	29	m2m.	49	6..	69	-42.m
10	..2/m	30	mmm.	50	-6..	70	-43m
11	2/m..	31	4/mmm	51	6/m..	71	m.m2
12	222	32	m.mm	52	622	72	4m.m
13	mm2	33	3..	53	6mm	73	4/mm.m
14	2mm	34	3.	54	-6m2	74	m-3m
15	m2m	35	-3..	55	-62m	75	-4m.2
16	mmm	35	-3.	56	6/mmm	76	.-3m
17	4..	37	3.2	57	.3.	77	.m.mm
18	-4..	38	32.	58	222..	78	<i>not used</i>
19	4/m..	39	.2	59	23.	79	<i>not used</i>
20	222.	40	32	60	mm2..		

NOTES:

1. In practise of course, code 1 is never assigned to an atom in a special position.

2. These are the codes applicable for each crystal class:

Triclinic	codes 1-2
Monoclinic	codes 1-11
Orthorhombic	codes 1-16
Tetragonal	codes 1-11,17-32 (27 in total)
Trigonal	codes 1-4,6,7,9,10,33-48 (24 in total)
Hexagonal	codes 1-16,33,35,37,38,41,42,45,46,49-56 (32 in total)
Cubic	codes 1,4,5,7,8,11,17-19,22,25,57-77 (32 in total)

Table 3-2 : Point Group (Pseudo-Symmetry) Symbol codes for atoms in general positions : assigned by module XDLSDb and by user intervention

Code	Symbol	Code	Symbol	Code	Symbol	Code	Symbol
80	cyl	89	4	98	32	107	6/mmm
81	1	90	-4	99	3m	108	23
82	-1	91	4/m	100	-3m	109	m-3
83	2	92	422	101	6	110	432
84	m	93	4mm	102	-6	111	-43m
85	2/m	94	-42m	103	6/m	112	m-3m
86	222	95	4/mmm	104	622		
87	mm2	96	3	105	6mm		
88	mmm	97	-3	106	-6m2		

NOTES:

1. These symmetries comprise the 32 crystallographic point groups plus 'cyl', which indicates cylindrical symmetry, often assigned to H atoms. Atoms in general positions with no assigned pseudo-symmetry are given the symbol '1' (code=81).

Table 4-5 : Index Picking Rules of Site-Symmetric Spherical Harmonics [25]

Symmetry	Choice of axes	Indices of symmetric y_{imp} (λ, μ are integers) ¹	Multipole refinement keys in XD
1	Any	all (l, m, \pm)	10 111 11111 1111111 111111111
-1	Any	($2\lambda, m, \pm$)	10 000 11111 0000000 111111111
2	$2 \parallel z$	($l, 2\mu, \pm$)	10 001 10011 1001100 100110011
m	$m \perp z$	($l, l-2\mu, \pm$)	10 110 10011 0110011 100110011
2/m	$2 \parallel z, m \perp z$	($2\lambda, 2\mu, \pm$)	10 000 10011 0000000 100110011
222	$2 \parallel z, 2 \parallel y, (2 \parallel x)$	($2\lambda, 2\mu, +$), ($2\lambda+1, 2\mu, -$)	10 000 10010 0000100 100100010
mm2	$2 \parallel z, m \perp y, (m \perp x)$	($l, 2\mu, +$)	10 001 10010 1001000 100100010
mmm	$m \perp z, m \perp y, m \perp x$	($2\lambda, 2\mu, +$)	10 000 10010 0000000 100100010
4	$4 \parallel z$	($l, 4\mu, \pm$)	10 001 10000 1000000 100000011
-4	$-4 \parallel z$	($2\lambda, 4\mu, \pm$), ($2\lambda+1, 4\mu+2, \pm$)	10 000 10000 0001100 100000011
4/m	$4 \parallel z, m \perp z$	($2\lambda, 4\mu, \pm$)	10 000 10000 0000000 100000011
422	$4 \parallel z, 2 \parallel y, (2 \parallel x)$	($2\lambda, 4\mu, +$), ($2\lambda+1, 4\mu, -$)	10 000 10000 0000000 100000010
4mm	$4 \parallel z, m \perp y, (m \perp x)$	($l, 4\mu, +$)	10 001 10000 1000000 100000010
-42m	$-4 \parallel z, 2 \parallel x$	($2\lambda, 4\mu, +$), ($2\lambda+1, 4\mu+2, -$)	10 000 10000 0000100 100000010
-4m2	$-4 \parallel z, m \perp y$	($2\lambda, 4\mu, +$), ($2\lambda+1, 4\mu+2, +$)	10 000 10000 0001000 100000010
4/mmm	$4 \parallel z, m \perp z, (m \perp x),$	($2\lambda, 4\mu, +$)	10 000 10000 0000000 100000010
3	$3 \parallel z$	($l, 3\mu, \pm$)	10 001 10000 1000011 100001100
-3	$-3 \parallel z$	($2\lambda, 3\mu, \pm$)	10 000 10000 0000000 100001100
32	(a) $3 \parallel z, 2 \parallel y$ (b) $3 \parallel z, 2 \parallel x$	($2\lambda, 3\mu, +$), ($2\lambda+1, 3\mu, -$) ($3\mu+2j, 3\mu, +$) ($3\mu+2j+1, 3\mu, -$)	10 000 10000 0000001 100001000 10 000 10000 0000010 100000100
3m	(a) $3 \parallel z, m \perp y$ (b) $3 \parallel z, m \perp x$	($l, 3\mu, +$) ($l, 6\mu, +$), ($l, 6\mu+3, -$)	10 001 10000 1000010 100001000 10 001 10000 1000001 100000100
-3m	(a) $-3 \parallel z, m \perp y$ (b) $-3 \parallel z, m \perp x$	($2\lambda, 3\mu, +$) ($2\lambda, 6\mu, +$), ($2\lambda, 6\mu+3, -$)	10 000 10000 0000000 100001000 10 000 10000 0000000 100000100
6	$6 \parallel z$	($l, 6\mu, \pm$)	10 001 10000 1000000 100000000
-6	$-6 \parallel z = (3 \parallel z, m \perp z)$	($2\lambda, 6\mu, \pm$), ($2\lambda+1, 6\mu+3, \pm$)	10 000 10000 0000011 100000000
6/m	$6 \parallel z, m \perp y, 2 \parallel y, (2 \parallel x)$	($2\lambda, 6\mu, \pm$)	10 000 10000 0000000 100000000
622	$6 \parallel z, 2 \parallel y, (2 \parallel x)$	($2\lambda, 6\mu, +$), ($2\lambda+1, 6\mu, -$)	10 000 10000 0000000 100000000
6mm	$6 \parallel z, m \perp y, (m \perp x)$	($l, 6\mu, +$)	10 001 10000 1000000 100000000
-6m2	$-6 \parallel z, m \perp y, (2 \parallel x)$	($2\lambda, 6\mu, +$), ($2\lambda+1, 6\mu+3, +$)	10 000 10000 0000010 100000000
-62m	$-6 \parallel z, m \perp y, (2 \parallel y)$	($2\lambda, 6\mu, +$), ($2\lambda+1, 6\mu+3, -$)	10 000 10000 0000001 100000000
6/mmm	$6 \parallel z, m \perp z, m \perp y, (m \perp x)$	($2\lambda, 6\mu, +$)	10 000 10000 0000000 100000000

1. Note that $m = -0$ is antisymmetric, while $m = +0$ or ± 0 is symmetric. For instance, with symmetry 222, the picking rule ($2\lambda, 2\mu, +$) tells us that $y_{2,0}$ & $y_{4,0}$ are symmetric, while the picking rule ($2\lambda+1, 2\mu, -$) tells us that $y_{1,0}$ ($\lambda = 0, \mu = 0$) or $y_{3,0}$ ($\lambda = 1, \mu = 0$) are antisymmetric, while $y_{3,-2}$ ($\lambda = 1, \mu = 1$) is symmetric.

Table 4-6 : Site Symmetry Table Giving the Key to Tables 4-7 to 4-9 (Hex indicates hexagonal axes).

Point Symmetry at Special Position				Position x,y,z	Cross reference key		
Symmetry Axes		Point Group Generators			4-7	4-8	4-9
m3̄m		4[0,0,1]	3[1,1,1] 1̄	0,0,0	B1	C0	D1
4̄3m		4̄[0,0,1]	3[1,1,1]	0,0,0	B1	C1	D1
432		4[0,0,1]	3[1,1,1]	0,0,0	B1	C0	D1
m3̄		3[1,1,1]	2[0,0,1] 1̄	0,0,0	B1	C0	D1
23		3[1,1,1]	2[0,0,1]	0,0,0	B1	C1	D1
6/mmm	Hex	6[0,0,1]	2[1,0,0] 1̄	0,0,0	B9	C0	D2
6̄m2	Hex	6̄[0,0,1]	2[1,0,0]	0,0,0	B9	C9	D2
6̄m2	Hex	6̄[0,0,1]	2[1,2,0]	0,0,0	B9	C10	D2
6mm	Hex	6[0,0,1]	2̄[1,0,0]	0,0,z	B9	C19	D2
622	Hex	6[0,0,1]	2[1,0,0]	0,0,0	B9	C0	D2
6/m	Hex	6[0,0,1]	1̄	0,0,0	B9	C0	D2
6̄	Hex	6̄[0,0,1]		0,0,0	B9	C20	D2
6	Hex	6[0,0,1]		0,0,z	B9	C19	D2
4/mmm		4[0,0,1]	2[1,0,0] 1̄	0,0,0	B2	C0	D3
4/mmm		4[0,1,0]	2[0,0,1] 1̄	0,0,0	B3	C0	D4
4/mmm		4[1,0,0]	2[0,1,0] 1̄	0,0,0	B4	C0	D5
4̄2m		4̄[0,0,1]	2[1,0,0]	0,0,0	B2	C1	D3
4̄2m		4̄[0,0,1]	2[1,1,0]	0,0,0	B2	C2	D3
4̄2m		4̄[0,1,0]	2[0,0,1]	0,0,0	B3	C1	D4
4̄2m		4̄[0,1,0]	2[1,0,1]	0,0,0	B3	C3	D4
4̄2m		4̄[1,0,0]	2[0,1,0]	0,0,0	B4	C1	D5
4̄2m		4̄[1,0,0]	2[0,1,1]	0,0,0	B4	C4	D5
4mm		4[0,0,1]	2̄[1,0,0]	0,0,z	B2	C13	D3
4mm		4[0,1,0]	2̄[0,0,1]	0,y,0	B3	C14	D4
4mm		4[1,0,0]	2̄[0,1,0]	x,0,0	B4	C15	D5
422		4[0,0,1]	2[1,0,0]	0,0,0	B2	C0	D3
422		4[0,1,0]	2[0,0,1]	0,0,0	B3	C0	D4
422		4[1,0,0]	2[0,1,0]	0,0,0	B4	C0	D5
4/m		4[0,0,1]	1̄	0,0,0	B2	C0	D12
4/m		4[0,1,0]	1̄	0,0,0	B3	C0	D13
4/m		4[1,0,0]	1̄	0,0,0	B4	C0	D14
4̄		4̄[0,0,1]		0,0,0	B2	C16	D12
4̄		4̄[0,1,0]		0,0,0	B3	C17	D13
4̄		4̄[1,0,0]		0,0,0	B4	C18	D14
4		4[0,0,1]		0,0,z	B2	C13	D12
4		4[0,1,0]		0,y,0	B3	C14	D13
4		4[1,0,0]		x,0,0	B4	C15	D14
3̄m		3[1,1,1]	2[1,1̄,0] 1̄	0,0,0	B5	C0	D6
3̄m		3[1,1,1̄]	2[1,1̄,0] 1̄	0,0,0	B6	C0	D7
3̄m		3[1,1̄,1]	2[1,1,0] 1̄	0,0,0	B7	C0	D8
3̄m		3[1̄,1,1]	2[1,1,0] 1̄	0,0,0	B8	C0	D9
3̄m	Hex	3[0,0,1]	2[1,0,0] 1̄	0,0,0	B9	C0	D10
3̄m	Hex	3[0,0,1]	2[1,2,0] 1̄	0,0,0	B9	C0	D11
3m		3[1,1,1]	2̄[1,1̄,0]	x,x,x	B5	C33	D6
3m		3[1,1,1̄]	2̄[1,1̄,0]	x,x,x̄	B6	C34	D7
3m		3[1,1̄,1]	2̄[1,1,0]	x,x̄,x	B7	C35	D8
3m		3[1̄,1,1]	2̄[1,1,0]	x̄,x,x	B8	C36	D9
3m	Hex	3[0,0,1]	2̄[1,0,0]	0,0,z	B9	C37	D10
3m	Hex	3[0,0,1]	2̄[1,2,0]	0,0,z	B9	C38	D11
32		3[1,1,1]	2[1,1̄,0]	0,0,0	B5	C5	D6

Table 4-6 : (cont)

Point Symmetry at Special Position				Position x,y,z	Cross reference key			
Symmetry Axes	Point Group Generators				4-7	4-8	4-9	
32	Hex	3[1,1, $\bar{1}$]	2[1, $\bar{1}$,0]	0,0,0	B6	C6	D7	
32		3[1, $\bar{1}$,1]	2[1,1,0]	0,0,0	B7	C7	D8	
32		3[$\bar{1}$,1,1]	2[1,1,0]	0,0,0	B8	C8	D9	
32		3[0,0,1]	2[1,0,0]	0,0,0	B9	C9	D10	
32		3[0,0,1]	2[1,2,0]	0,0,0	B9	C10	D11	
$\bar{3}$	Hex	$\bar{3}$ [1,1,1]		0,0,0	B5	C0	D15	
$\bar{3}$		$\bar{3}$ [1,1, $\bar{1}$]		0,0,0	B6	C0	D16	
$\bar{3}$		$\bar{3}$ [1, $\bar{1}$,1]		0,0,0	B7	C0	D17	
$\bar{3}$		$\bar{3}$ [$\bar{1}$,1,1]		0,0,0	B8	C0	D18	
$\bar{3}$		$\bar{3}$ [0,0,1]		0,0,0	B9	C0	D19	
3	Hex	3[1,1,1]		x,x,x	B5	C54	D15	
3		3[1,1, $\bar{1}$]		x,x, \bar{x}	B6	C55	D16	
3		3[1, $\bar{1}$,1]		x, \bar{x} ,x	B7	C56	D17	
3		3[$\bar{1}$,1,1]		\bar{x} ,x,x	B8	C57	D18	
3		3[0,0,1]		0,0,z	B9	C58	D19	
mmm	Hex	2[0,0,1]	2[1,0,0]	$\bar{1}$	0,0,0	B10	C0	D20
mmm		2[0,0,1]	2[1,1,0]	$\bar{1}$	0,0,0	B11	C0	D21
mmm		2[0,1,0]	2[1,0,1]	$\bar{1}$	0,0,0	B12	C0	D22
mmm		2[1,0,0]	2[0,1,1]	$\bar{1}$	0,0,0	B13	C0	D23
mmm		2[0,0,1]	2[1,0,0]	$\bar{1}$	0,0,0	B14	C0	D24
mmm		2[0,0,1]	2[1,1,0]	$\bar{1}$	0,0,0	B11	C0	D21
mmm		2[0,0,1]	2[0,1,0]	$\bar{1}$	0,0,0	B15	C0	D25
mm		2[0,0,1]	$\bar{2}$ [1,0,0]		0,0,z	B10	C21	D20
mm		2[0,0,1]	$\bar{2}$ [1,1,0]		0,0,z	B11	C22	D21
mm		2[0,1,0]	$\bar{2}$ [0,0,1]		0,y,0	B10	C23	D20
mm		2[0,1,0]	$\bar{2}$ [1,0,1]		0,y,0	B12	C24	D22
mm		2[1,0,0]	$\bar{2}$ [0,0,1]		x,0,0	B10	C25	D20
mm		2[1,0,0]	$\bar{2}$ [0,1,1]		x,0,0	B13	C26	D23
mm		2[1,1,0]	$\bar{2}$ [0,0,1]		x,x,0	B11	C27	D21
mm		2[1, $\bar{1}$,0]	$\bar{2}$ [0,0,1]		x, \bar{x} ,0	B11	C28	D21
mm		2[1,0,1]	$\bar{2}$ [0,1,0]		x,0,x	B12	C29	D22
mm	2[1,0, $\bar{1}$]	$\bar{2}$ [0,1,0]		x,0, \bar{x}	B12	C30	D22	
mm	2[0,1,1]	$\bar{2}$ [1,0,0]		0,y,y	B13	C31	D23	
mm	2[0,1, $\bar{1}$]	$\bar{2}$ [1,0,0]		0,y, \bar{y}	B13	C32	D23	
mm	Hex	2[0,0,1]	$\bar{2}$ [1,0,0]	0,0,z	B14	C40	D24	
mm	Hex	2[0,0,1]	$\bar{2}$ [1,1,0]	0,0,z	B11	C22	D21	
mm	Hex	2[0,0,1]	$\bar{2}$ [0,1,0]	0,0,z	B15	C39	D25	
mm	Hex	2[1,0,0]	$\bar{2}$ [0,0,1]	x,0,0	B14	C41	D24	
mm	Hex	2[2,1,0]	$\bar{2}$ [0,0,1]	2x,x,0	B15	C42	D25	
mm	Hex	2[1,1,0]	$\bar{2}$ [0,0,1]	x,x,0	B11	C27	D21	
mm	Hex	2[1,2,0]	$\bar{2}$ [0,0,1]	x,2x,0	B14	C43	D24	
mm	Hex	2[0,1,0]	$\bar{2}$ [0,0,1]	0,y,0	B15	C44	D25	
mm	Hex	2[1, $\bar{1}$,0]	$\bar{2}$ [0,0,1]	x, \bar{x} ,0	B11	C28	D21	
222	Hex	2[0,0,1]	2[1,0,0]	0,0,0	B10	C1	D20	
222		2[0,0,1]	2[1,1,0]	0,0,0	B11	C2	D21	
222		2[0,1,0]	2[1,0,1]	0,0,0	B12	C3	D22	
222		2[1,0,0]	2[0,1,1]	0,0,0	B13	C4	D23	
222		2[0,0,1]	2[1,0,0]	0,0,0	B14	C11	D24	
222		2[0,0,1]	2[1,1,0]	0,0,0	B11	C2	D21	
222		2[0,0,1]	2[0,1,0]	0,0,0	B15	C12	D25	
2/m			2[0,0,1]	$\bar{1}$	0,0,0	B16	C0	D26

Table 4-6 : (cont)

Point Symmetry at Special Position		Position x,y,z	Cross reference key		
Symmetry Axes	Point Group Generators		4-7	4-8	4-9
2/m	2[0,1,0] $\bar{1}$	0,0,0	B17	C0	D27
2/m	2[1,0,0] $\bar{1}$	0,0,0	B18	C0	D28
2/m	2[1,1,0] $\bar{1}$	0,0,0	B19	C0	D29
2/m	2[1, $\bar{1}$,0] $\bar{1}$	0,0,0	B20	C0	D30
2/m	2[1,0,1] $\bar{1}$	0,0,0	B21	C0	D31
2/m	2[1,0, $\bar{1}$] $\bar{1}$	0,0,0	B22	C0	D32
2/m	2[0,1,1] $\bar{1}$	0,0,0	B23	C0	D33
2/m	2[0,1, $\bar{1}$] $\bar{1}$	0,0,0	B24	C0	D34
2/m Hex	2[0,0,1] $\bar{1}$	0,0,0	B16	C0	D26
2/m Hex	2[1,0,0] $\bar{1}$	0,0,0	B25	C0	D35
2/m Hex	2[2,1,0] $\bar{1}$	0,0,0	B26	C0	D36
2/m Hex	2[1,1,0] $\bar{1}$	0,0,0	B19	C0	D29
2/m Hex	2[1,2,0] $\bar{1}$	0,0,0	B27	C0	D37
2/m Hex	2[0,1,0] $\bar{1}$	0,0,0	B28	C0	D38
2/m Hex	2[1, $\bar{1}$,0] $\bar{1}$	0,0,0	B20	C0	D30
m	$\bar{2}$ [0,1,0]	x,0,z	B17	C64	D27
m	$\bar{2}$ [1,0,0]	0,y,z	B18	C65	D28
m	$\bar{2}$ [1,1,0]	x, \bar{x} ,z	B19	C66	D29
m	$\bar{2}$ [1, $\bar{1}$,0]	x,x,z	B20	C67	D30
m	$\bar{2}$ [1,0,1]	x,y, \bar{x}	B21	C68	D31
m	$\bar{2}$ [1,0, $\bar{1}$] $\bar{1}$	x,y,x	B22	C69	D32
m	$\bar{2}$ [0,1,1]	x,y, \bar{y}	B23	C70	D33
m	$\bar{2}$ [0,1, $\bar{1}$] $\bar{1}$	x,y,y	B24	C71	D34
m Hex	$\bar{2}$ [0,0,1]	x,y,0	B16	C63	D26
m Hex	$\bar{2}$ [1,0,0]	x,2x,z	B25	C72	D35
m Hex	$\bar{2}$ [2,1,0]	0,y,z	B26	C73	D36
m Hex	$\bar{2}$ [1,1,0]	x, \bar{x} ,z	B19	C66	D29
m Hex	$\bar{2}$ [1,2,0]	x,0,z	B27	C74	D37
m Hex	$\bar{2}$ [0,1,0]	2x,x,z	B28	C75	D38
m Hex	$\bar{2}$ [1, $\bar{1}$,0]	x,x,z	B20	C67	D30
2	2[0,0,1]	0,0,z	B16	C45	D26
2	2[0,1,0]	0,y,0	B17	C46	D27
2	2[1,0,0]	x,0,0	B18	C47	D28
2	2[1,1,0]	x,x,0	B19	C48	D29
2	2[1, $\bar{1}$,0]	x, \bar{x} ,0	B20	C49	D30
2	2[1,0,1]	x,0,x	B21	C50	D31
2	2[1,0, $\bar{1}$] $\bar{1}$	x,0, \bar{x}	B22	C51	D32
2	2[0,1,1]	0,y,y	B23	C52	D33
2	2[0,1, $\bar{1}$] $\bar{1}$	0,y, \bar{y}	B24	C53	D34
2 Hex	2[0,0,1]	0,0,z	B16	C45	D26
2 Hex	2[1,0,0]	x,0,0	B25	C59	D35
2 Hex	2[2,1,0]	2x,x,0	B26	C60	D36
2 Hex	2[1,1,0]	x,x,0	B19	C48	D29
2 Hex	2[1,2,0]	x,2x,0	B27	C61	D37
2 Hex	2[0,1,0]	0,y,0	B28	C62	D38
2 Hex	2[1, $\bar{1}$,0]	x, \bar{x} ,0	B20	C49	D30
$\bar{1}$	$\bar{1}$	0,0,0	B29	C0	D39
$\bar{1}$ Hex	$\bar{1}$	0,0,0	B29	C0	D39
1	1	x,y,z	B29	C76	D39
1 Hex	1	x,y,z	B29	C76	D39

Table 4-7 : Site symmetry restrictions on coefficients of the U^j tensor.

Cross reference from Table 4-6	Number of indep. variables	Symbols and coefficient indices					
		A	B	C	D	E	F
		(1) (1)	(2) (2)	(3) (3)	(1) (2)	(1) (3)	(2) (3)
B1	1	A	A	A	0	0	0
B2	2	A	A	C	0	0	0
B3	2	A	B	A	0	0	0
B4	2	A	B	B	0	0	0
B5	2	A	A	A	D	D	D
B6	2	A	A	A	D	-D	-D
B7	2	A	A	A	D	-D	D
B8	2	A	A	A	D	D	-D
B9	2	A	A	C	A/2	0	0
B10	3	A	B	C	0	0	0
B11	3	A	A	C	D	0	0
B12	3	A	B	A	0	E	0
B13	3	A	B	B	0	0	F
B14	3	A	B	C	B/2	0	0
B15	3	A	B	C	A/2	0	0
B16	4	A	B	C	D	0	0
B17	4	A	B	C	0	E	0
B18	4	A	B	C	0	0	F
B19	4	A	A	C	D	E	-E
B20	4	A	A	C	D	E	E
B21	4	A	B	A	D	E	-D
B22	4	A	B	A	D	E	D
B23	4	A	B	B	D	-D	F
B24	4	A	B	B	D	D	F
B25	4	A	B	C	B/2	F/2	F
B26	4	A	B	C	A/2	0	F
B27	4	A	B	C	B/2	E	0
B28	4	A	B	C	A/2	E	E/2
B29	6	A	B	C	D	E	F

Table 4-8 : Site symmetry restrictions on third-order Gram-Charlier coefficients C_{ijk} .

Cross reference from Table 4-6	Number of indep. variables	Symbols and coefficient indices									
		A	B	C	D	E	F	G	H	I	J
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(2)	(2)	(1)
		(1)	(2)	(3)	(1)	(2)	(1)	(3)	(2)	(3)	(2)
		(1)	(2)	(3)	(2)	(2)	(3)	(3)	(3)	(3)	(3)
C0	0	0	0	0	0	0	0	0	0	0	0
C1	1	0	0	0	0	0	0	0	0	0	J
C2	1	0	0	0	0	0	F	0	-F	0	0
C3	1	0	0	0	D	0	0	0	0	-D	0
C4	1	0	0	0	0	E	0	-E	0	0	0
C5	1	0	0	0	D	-D	-D	D	D	-D	0
C6	1	0	0	0	D	-D	D	D	-D	-D	0
C7	1	0	0	0	D	D	D	-D	-D	-D	0
C8	1	0	0	0	D	D	-D	-D	D	-D	0
C9	1	0	0	0	D	D	0	0	0	0	0
C10	1	A	-A	0	A/2	-A/2	0	0	0	0	0
C11	1	0	0	0	0	0	F	0	0	0	F
C12	1	0	0	0	0	0	0	0	H	0	H
C13	2	0	0	C	0	0	F	0	F	0	0
C14	2	0	B	0	D	0	0	0	0	D	0
C15	2	A	0	0	0	E	0	E	0	0	0
C16	2	0	0	0	0	0	F	0	-F	0	J
C17	2	0	0	0	D	0	0	0	0	-D	J
C18	2	0	0	0	0	E	0	-E	0	0	J
C19	2	0	0	C	0	0	F	0	F	0	F/2
C20	2	A	-A	0	D	D-A	0	0	0	0	0
C21	3	0	0	C	0	0	F	0	H	0	0
C22	3	0	0	C	0	0	F	0	F	0	J
C23	3	0	B	0	D	0	0	0	0	I	0
C24	3	0	B	0	D	0	0	0	0	D	J
C25	3	A	0	0	0	E	0	G	0	0	0
C26	3	A	0	0	0	E	0	E	0	0	J
C27	3	A	A	0	D	D	0	G	0	G	0
C28	3	A	-A	0	D	-D	0	G	0	-G	0
C29	3	A	0	A	0	E	F	F	E	0	0
C30	3	A	0	-A	0	E	F	-F	-E	0	0
C31	3	0	B	B	D	0	D	0	H	H	0
C32	3	0	B	-B	D	0	-D	0	H	-H	0
C33	3	A	A	A	D	D	D	D	D	D	J
C34	3	A	A	-A	D	D	-D	D	-D	D	J
C35	3	A	-A	A	D	-D	-D	-D	-D	D	J
C36	3	A	-A	-A	D	-D	D	-D	D	D	J
C37	3	A	-A	C	A/2	-A/2	F	0	F	0	F/2
C38	3	0	0	C	D	D	F	0	F	0	F/2
C39	3	0	0	C	0	0	F	0	H	0	F/2
C40	3	0	0	C	0	0	F	0	H	0	H/2
C41	3	A	0	0	D	D	0	G	0	0	0
C42	3	A	B	0	A/2	A/6+2B/3	0	G	0	G/2	0
C43	3	A	B	0	B/6+2A/3	B/2	0	1/2	0	I	0
C44	3	0	B	0	D	D	0	0	0	I	0
C45	4	0	0	C	0	0	F	0	H	0	J
C46	4	0	B	0	D	0	0	0	0	I	J
C47	4	A	0	0	0	E	0	G	0	0	J
C48	4	A	A	0	D	D	F	G	-F	G	0
C49	4	A	-A	0	D	-D	F	G	-F	-G	0

Appendix

Table 4-8 : (cont)

Cross reference from Table 4-6	Number of indep. variables	Symbols and coefficient indices									
		A	B	C	D	E	F	G	H	I	J
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(2)	(2)	(1)
		(1)	(2)	(3)	(1)	(2)	(1)	(3)	(2)	(3)	(2)
		(1)	(2)	(3)	(2)	(2)	(3)	(3)	(3)	(3)	(3)
C50	4	A	0	A	D	E	F	F	E	-D	0
C51	4	A	0	-A	D	E	F	-F	-E	-D	0
C52	4	0	B	B	D	E	D	-E	H	H	0
C53	4	0	B	-B	D	E	-D	-E	H	-H	0
C54	4	A	A	A	D	E	E	D	D	E	J
C55	4	A	A	-A	D	E	-E	D	-D	E	J
C56	4	A	-A	A	D	E	E	-D	-D	-E	J
C57	4	A	-A	-A	D	E	-E	-D	D	-E	J
C58	4	A	-A	C	D	D-A	F	0	F	0	F/2
C59	4	A	0	0	D	D	F	G	0	0	F
C60	4	A	B	0	A/2	A/6+2B/3	0	G	H	G/2	H
C61	4	A	B	0	B/6+2A/3	B/2	F	I/2	0	I	F
C62	4	0	B	0	D	D	0	0	H	I	H
C63	6	A	B	0	D	E	0	G	0	I	0
C64	6	A	0	C	0	E	F	G	H	0	0
C65	6	0	B	C	D	0	F	0	H	I	0
C66	6	A	-A	C	D	-D	F	G	F	-G	J
C67	6	A	A	C	D	D	F	G	F	G	J
C68	6	A	B	-A	D	E	F	-F	-E	D	J
C69	6	A	B	A	D	E	F	F	E	D	J
C70	6	A	B	-B	D	E	-D	E	H	-H	J
C71	6	A	B	B	D	E	D	E	H	H	J
C72	6	A	B	C	B/6+2A/3	B/2	F	I/2	H	I	H/2
C73	6	0	B	C	D	D	F	0	H	I	F/2
C74	6	A	0	C	D	D	F	G	H	0	H/2
C75	6	A	B	C	A/2	A/6+2B/3	F	G	H	G/2	F/2
C76	10	A	B	C	D	E	F	G	H	I	J

Table 4-9 : Site symmetry restrictions on fourth-order Gram-Charlier coefficients D_{ijkl} .

Cross reference from Table 4-6	Number of indep. variables	Symbols and coefficient indices															
		A	B	C	D	E	F	G	H	I	J	K	L	M	N	P	
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(2)	(2)	(1)	(1)	(2)	(1)	(1)	(1)	
		(1)	(2)	(3)	(1)	(2)	(1)	(3)	(2)	(3)	(1)	(1)	(2)	(1)	(2)	(2)	
		(1)	(2)	(3)	(1)	(2)	(1)	(3)	(2)	(3)	(2)	(3)	(3)	(2)	(2)	(3)	
D1	2	A	A	A	0	0	0	0	0	J	J	J	0	0	0		
D2	3	A	A	C	A/2	A/2	0	0	0	A/2	K	K	0	0	K/2		
D3	3	A	A	C	0	0	0	0	0	J	K	K	0	0	0		
D4	4	A	B	A	0	0	0	0	0	J	K	J	0	0	0		
D5	4	A	B	B	0	0	0	0	0	J	J	L	0	0	0		
D6	4	A	A	A	D	D	D	D	D	J	J	J	M	M	M		
D7	4	A	A	A	D	D	-D	-D	-D	J	J	J	M	M	-M		
D8	4	A	A	A	D	D	-D	-D	D	J	J	J	M	-M	M		
D9	4	A	A	A	D	D	D	D	-D	J	J	J	M	-M	-M		
D10	4	A	A	C	A/2	A/2	F	0	-F	A/2	K	K	F/2	-F/2	K/2		
D11	4	A	A	C	A/2	A/2	0	0	0	A/2	K	K	M	M	K/2		
D12	5	A	A	C	D	-D	0	0	0	J	K	K	0	0	0		
D13	5	A	B	A	0	0	F	-F	0	J	K	J	0	0	0		
D14	5	A	B	B	0	0	0	0	H	-H	J	J	L	0	0		
D15	5	A	A	A	D	E	E	D	D	E	J	J	J	M	M		
D16	5	A	A	A	D	E	-E	-D	-D	-E	J	J	J	M	M		
D17	5	A	A	A	D	E	-E	-D	D	E	J	J	J	M	-M		
D18	5	A	A	A	D	E	E	D	-D	-E	J	J	J	M	-M		
D19	5	A	A	C	A/2	A/2	F	0	-F	A/2	K	K	M	M-F	K/2		
D20	6	A	B	C	0	0	0	0	0	J	K	L	0	0	0		
D21	6	A	A	C	D	D	0	0	0	J	K	K	0	0	P		
D22	6	A	B	A	0	0	F	F	0	J	K	J	0	N	0		
D23	6	A	B	B	0	0	0	0	H	H	J	J	L	M	0		
D24	6	A	B	C	D	B/2	0	0	0	B/6+2D/3	K	L	0	0	L/2		
D25	6	A	B	C	A/2	E	0	0	0	A/6+2E/3	K	L	0	0	K/2		
D26	9	A	B	C	D	E	0	0	0	J	K	L	0	0	P		
D27	9	A	B	C	0	0	F	G	0	J	K	L	0	N	0		
D28	9	A	B	C	0	0	0	0	H	I	J	K	L	M	0		
D29	9	A	A	C	D	D	F	G	-F	-G	J	K	K	M	-M		
D30	9	A	A	C	D	D	F	G	F	G	J	K	K	M	M		
D31	9	A	B	A	D	E	F	F	-E	-D	J	K	J	M	N		
D32	9	A	B	A	D	E	F	F	E	D	J	K	J	M	N		
D33	9	A	B	B	D	E	-D	-E	H	H	J	J	L	M	N		
D34	9	A	B	B	D	E	D	E	H	H	J	J	L	M	N		
D35	9	A	B	C	D	B/2	F	I/2	H	I	B/6+2D/3	K	L	H/6+2F/3	H/2		
D36	9	A	B	C	A/2	E	0	0	H	I	A/6+2E/3	K	L	M	M		
D37	9	A	B	C	D	B/2	F	G	0	0	B/6+2D/3	K	L	M	M		
D38	9	A	B	C	A/2	E	F	G	H	G/2	A/6+2E/3	K	L	F/2	F/6+2H/3		
D39	15	A	B	C	D	E	F	G	H	I	J	K	L	M	N		

