MSG No. 222.103 $P_In\bar{3}n$ [Type IV, cubic]

Table 1: Wyckoff site: 2a, site symmetry: m'-3'm'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,
		73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96]
2	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,
		49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72]

Table 2: Wyckoff site: 6b, site symmetry: 4/m'm'.m'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,2,3,8,9,10,13,14,73,74,75,80,81,82,85,86]
2	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[4,5,15,16,18,19,21,23,76,77,87,88,90,91,93,95]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[6,7,11,12,17,20,22,24,78,79,83,84,89,92,94,96]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[25,26,27,32,33,34,37,38,49,50,51,56,57,58,61,62]
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[28,29,39,40,42,43,45,47,52,53,63,64,66,67,69,71]
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[30,31,35,36,41,44,46,48,54,55,59,60,65,68,70,72]

Table 3: Wyckoff site: 8c, site symmetry: .-3m

No.	position	mapping
1	$[0, 0, 0]$	[1,17,18,25,41,42,60,62,64,84,86,88]
2	$\left[0, \frac{1}{2}, 0\right]$	[2,7,15,26,31,39,57,67,72,81,91,96]
3	$\left[0, 0, \frac{1}{2}\right]$	[3,4,11,27,28,35,58,68,69,82,92,93]
4	$\left[\frac{1}{2}, 0, 0\right]$	[5,6,13,29,30,37,56,70,71,80,94,95]
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[8,22,23,32,46,47,53,54,61,77,78,85]
6	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[9,19,24,33,43,48,50,55,63,74,79,87]
7	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[10,20,21,34,44,45,51,52,59,75,76,83]
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[12,14,16,36,38,40,49,65,66,73,89,90]

Table 4: Wyckoff site: 12d, site symmetry: -4m'.2'

No.	position	mapping
1	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[1,8,26,27,61,62,81,82]
2	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[2,3,25,32,57,58,85,86]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[4,16,43,47,66,69,77,87]
4	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[5,15,42,45,67,71,76,88]
5	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[6,11,41,48,68,70,79,84]
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[7,12,44,46,65,72,78,83]
7	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[9,10,37,38,50,51,73,80]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[13,14,33,34,49,56,74,75]
9	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[17,24,30,35,55,60,92,94]
10	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[18,21,29,39,52,64,91,95]
11	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[19,23,28,40,53,63,90,93]
12	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[20,22,31,36,54,59,89,96]

Table 5: Wyckoff site: 12e, site symmetry: 4m'.m'

No.	position	mapping
1	$\left[x, \frac{3}{4}, \frac{3}{4}\right]$	[1,2,3,8,81,82,85,86]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x\right]$	[4,16,19,23,77,87,90,93]
3	$\left[\frac{3}{4}, \frac{3}{4}, x\right]$	[5,15,18,21,76,88,91,95]
4	$\left[\frac{3}{4}, x, \frac{3}{4}\right]$	[6,11,17,24,79,84,92,94]
5	$\left[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}\right]$	[7,12,20,22,78,83,89,96]
6	$\left[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}\right]$	[9,10,13,14,73,74,75,80]
7	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[25,26,27,32,57,58,61,62]
8	$\left[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}\right]$	[28,40,43,47,53,63,66,69]
9	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[29,39,42,45,52,64,67,71]
10	$\left[\frac{1}{4}, -x, \frac{1}{4}\right]$	[30,35,41,48,55,60,68,70]
11	$\left[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}\right]$	[31,36,44,46,54,59,65,72]
12	$\left[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[33,34,37,38,49,50,51,56]

Table 6: Wyckoff site: 16f, site symmetry: .3m'

No.	position	mapping
1	$[x, x, x]$	[1,17,18,84,86,88]
2	$\left[x, \frac{1}{2} - x, x\right]$	[2,7,15,81,91,96]
3	$\left[x, x, \frac{1}{2} - x\right]$	[3,4,11,82,92,93]
4	$\left[\frac{1}{2} - x, x, x\right]$	[5,6,13,80,94,95]
5	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[8,22,23,77,78,85]
6	$\left[\frac{1}{2} - x, x, \frac{1}{2} - x\right]$	[9,19,24,74,79,87]
7	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x\right]$	[10,20,21,75,76,83]
8	$\left[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[12,14,16,73,89,90]
9	$[-x, -x, -x]$	[25,41,42,60,62,64]
10	$\left[-x, x + \frac{1}{2}, -x\right]$	[26,31,39,57,67,72]
11	$\left[-x, -x, x + \frac{1}{2}\right]$	[27,28,35,58,68,69]
12	$\left[x + \frac{1}{2}, -x, -x\right]$	[29,30,37,56,70,71]
13	$\left[-x, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[32,46,47,53,54,61]
14	$\left[x + \frac{1}{2}, -x, x + \frac{1}{2}\right]$	[33,43,48,50,55,63]
15	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -x\right]$	[34,44,45,51,52,59]
16	$\left[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[36,38,40,49,65,66]

Table 7: Wyckoff site: `24g`, site symmetry: `2m'm'..`

No.	position	mapping
1	$\left[x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[1,8,81,82]`
2	$\left[x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[2,3,85,86]`
3	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-x\right]$	`[4,16,77,87]`
4	$\left[\frac{1}{4},\ \frac{3}{4},\ x\right]$	`[5,15,76,88]`
5	$\left[\frac{3}{4},\ x,\ \frac{1}{4}\right]$	`[6,11,79,84]`
6	$\left[\frac{3}{4},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[7,12,78,83]`
7	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[9,10,73,80]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[13,14,74,75]`
9	$\left[\frac{1}{4},\ x,\ \frac{3}{4}\right]$	`[17,24,92,94]`
10	$\left[\frac{3}{4},\ \frac{1}{4},\ x\right]$	`[18,21,91,95]`
11	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-x\right]$	`[19,23,90,93]`
12	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[20,22,89,96]`
13	$\left[-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[25,32,57,58]`
14	$\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[26,27,61,62]`
15	$\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{1}{2}\right]$	`[28,40,53,63]`
16	$\left[\frac{3}{4},\ \frac{1}{4},\ -x\right]$	`[29,39,52,64]`
17	$\left[\frac{1}{4},\ -x,\ \frac{3}{4}\right]$	`[30,35,55,60]`
18	$\left[\frac{1}{4},\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[31,36,54,59]`
19	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[33,34,49,56]`
20	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[37,38,50,51]`
21	$\left[\frac{3}{4},\ -x,\ \frac{1}{4}\right]$	`[41,48,68,70]`
22	$\left[\frac{1}{4},\ \frac{3}{4},\ -x\right]$	`[42,45,67,71]`
23	$\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{1}{2}\right]$	`[43,47,66,69]`
24	$\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[44,46,65,72]`

Table 8: Wyckoff site: `24h`, site symmetry: `m'.2m'`

No.	position	mapping
1	$\left[\frac{3}{4},\ y,\ y\right]$	`[1,13,80,86]`
2	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y\right]$	`[2,10,75,81]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,9,74,82]`
4	$\left[y,\ y,\ \frac{3}{4}\right]$	`[4,18,88,93]`
5	$\left[\frac{1}{2}-y,\ y,\ \frac{3}{4}\right]$	`[5,19,87,95]`
6	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	`[6,20,83,94]`
7	$\left[y,\ \frac{3}{4},\ y\right]$	`[7,17,84,96]`
8	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{2}-y\right]$	`[8,14,73,85]`
9	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	`[11,22,78,92]`
10	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	`[12,24,79,89]`
11	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	`[15,23,77,91]`
12	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	`[16,21,76,90]`
13	$\left[\frac{1}{4},\ -y,\ -y\right]$	`[25,37,56,62]`
14	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -y\right]$	`[26,34,51,57]`
15	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	`[27,33,50,58]`

continued ...

Table 8

No.	position	mapping
16	$\left[-y,\ -y,\ \frac{1}{4}\right]$	[28,42,64,69]
17	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	[29,43,63,71]
18	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[30,44,59,70]
19	$\left[-y,\ \frac{1}{4},\ -y\right]$	[31,41,60,72]
20	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	[32,38,49,61]
21	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[35,46,54,68]
22	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[36,48,55,65]
23	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[39,47,53,67]
24	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[40,45,52,66]

Table 9: Wyckoff site: 48i, site symmetry: ..2'

No.	position	mapping
1	$[0,\ y,\ -y]$	[1,62]
2	$\left[0,\ y+\frac{1}{2},\ y\right]$	[2,57]
3	$\left[0,\ -y,\ \frac{1}{2}-y\right]$	[3,58]
4	$\left[-y,\ y,\ \frac{1}{2}\right]$	[4,69]
5	$\left[y+\frac{1}{2},\ y,\ 0\right]$	[5,71]
6	$\left[\frac{1}{2}-y,\ 0,\ -y\right]$	[6,70]
7	$\left[y,\ \frac{1}{2},\ -y\right]$	[7,72]
8	$\left[0,\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[8,61]
9	$\left[\frac{1}{2},\ y,\ y+\frac{1}{2}\right]$	[9,50]
10	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -y\right]$	[10,51]
11	$\left[y,\ 0,\ y+\frac{1}{2}\right]$	[11,68]
12	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[12,65]
13	$\left[\frac{1}{2},\ -y,\ y\right]$	[13,56]
14	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[14,49]
15	$\left[-y,\ \frac{1}{2}-y,\ 0\right]$	[15,67]
16	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[16,66]
17	$[-y,\ 0,\ y]$	[17,60]
18	$[y,\ -y,\ 0]$	[18,64]
19	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{2}\right]$	[19,63]
20	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y\right]$	[20,59]
21	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ 0\right]$	[21,52]
22	$\left[-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[22,54]
23	$\left[y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[23,53]
24	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	[24,55]
25	$[0,\ -y,\ y]$	[25,86]
26	$\left[0,\ \frac{1}{2}-y,\ -y\right]$	[26,81]
27	$\left[0,\ y,\ y+\frac{1}{2}\right]$	[27,82]
28	$\left[y,\ -y,\ \frac{1}{2}\right]$	[28,93]
29	$\left[\frac{1}{2}-y,\ -y,\ 0\right]$	[29,95]
30	$\left[y+\frac{1}{2},\ 0,\ y\right]$	[30,94]
31	$\left[-y,\ \frac{1}{2},\ y\right]$	[31,96]

continued ...

Table 9

No.	position	mapping
32	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[32,85]
33	$\left[\frac{1}{2},\, -y,\, \frac{1}{2}-y\right]$	[33,74]
34	$\left[\frac{1}{2},\, y+\frac{1}{2},\, y\right]$	[34,75]
35	$\left[-y,\, 0,\, \frac{1}{2}-y\right]$	[35,92]
36	$\left[y+\frac{1}{2},\, \frac{1}{2},\, \frac{1}{2}-y\right]$	[36,89]
37	$\left[\frac{1}{2},\, y,\, -y\right]$	[37,80]
38	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, y+\frac{1}{2}\right]$	[38,73]
39	$\left[y,\, y+\frac{1}{2},\, 0\right]$	[39,91]
40	$\left[\frac{1}{2}-y,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[40,90]
41	$[y,\, 0,\, -y]$	[41,84]
42	$[-y,\, y,\, 0]$	[42,88]
43	$\left[y+\frac{1}{2},\, y,\, \frac{1}{2}\right]$	[43,87]
44	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, -y\right]$	[44,83]
45	$\left[y+\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	[45,76]
46	$\left[y,\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[46,78]
47	$\left[-y,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[47,77]
48	$\left[\frac{1}{2}-y,\, 0,\, y+\frac{1}{2}\right]$	[48,79]

Table 10: Wyckoff site: 48j, site symmetry: m'..

No.	position	mapping
1	$\left[\frac{3}{4},\, y,\, z\right]$	[1,80]
2	$\left[\frac{3}{4},\, \frac{1}{2}-z,\, y\right]$	[2,75]
3	$\left[\frac{3}{4},\, z,\, \frac{1}{2}-y\right]$	[3,74]
4	$\left[z,\, y,\, \frac{3}{4}\right]$	[4,88]
5	$\left[\frac{1}{2}-z,\, y,\, \frac{3}{4}\right]$	[5,87]
6	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, z\right]$	[6,83]
7	$\left[y,\, \frac{3}{4},\, z\right]$	[7,84]
8	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[8,73]
9	$\left[\frac{3}{4},\, y,\, \frac{1}{2}-z\right]$	[9,82]
10	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, z\right]$	[10,81]
11	$\left[y,\, \frac{3}{4},\, \frac{1}{2}-z\right]$	[11,78]
12	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, \frac{1}{2}-z\right]$	[12,79]
13	$\left[\frac{3}{4},\, z,\, y\right]$	[13,86]
14	$\left[\frac{3}{4},\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[14,85]
15	$\left[z,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[15,77]
16	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[16,76]
17	$\left[z,\, \frac{3}{4},\, y\right]$	[17,96]
18	$\left[y,\, z,\, \frac{3}{4}\right]$	[18,93]
19	$\left[\frac{1}{2}-y,\, z,\, \frac{3}{4}\right]$	[19,95]
20	$\left[\frac{1}{2}-z,\, \frac{3}{4},\, y\right]$	[20,94]
21	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, \frac{3}{4}\right]$	[21,90]
22	$\left[z,\, \frac{3}{4},\, \frac{1}{2}-y\right]$	[22,92]
23	$\left[y,\, \frac{1}{2}-z,\, \frac{3}{4}\right]$	[23,91]

continued ...

Table 10

No.	position	mapping
24	$\left[\frac{1}{2}-z,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[24,89]
25	$\left[\frac{1}{4},\ -y,\ -z\right]$	[25,56]
26	$\left[\frac{1}{4},\ z+\frac{1}{2},\ -y\right]$	[26,51]
27	$\left[\frac{1}{4},\ -z,\ y+\frac{1}{2}\right]$	[27,50]
28	$\left[-z,\ -y,\ \frac{1}{4}\right]$	[28,64]
29	$\left[z+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	[29,63]
30	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[30,59]
31	$\left[-y,\ \frac{1}{4},\ -z\right]$	[31,60]
32	$\left[\frac{1}{4},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32,49]
33	$\left[\frac{1}{4},\ -y,\ z+\frac{1}{2}\right]$	[33,58]
34	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -z\right]$	[34,57]
35	$\left[-y,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[35,54]
36	$\left[y+\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[36,55]
37	$\left[\frac{1}{4},\ -z,\ -y\right]$	[37,62]
38	$\left[\frac{1}{4},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[38,61]
39	$\left[-z,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[39,53]
40	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[40,52]
41	$\left[-z,\ \frac{1}{4},\ -y\right]$	[41,72]
42	$\left[-y,\ -z,\ \frac{1}{4}\right]$	[42,69]
43	$\left[y+\frac{1}{2},\ -z,\ \frac{1}{4}\right]$	[43,71]
44	$\left[z+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[44,70]
45	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[45,66]
46	$\left[-z,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[46,68]
47	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[47,67]
48	$\left[z+\frac{1}{2},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[48,65]

Table 11: Wyckoff site: 48k, site symmetry: ..m'

No.	position	mapping
1	$[x,\ x,\ z]$	[1,84]
2	$\left[x,\ \frac{1}{2}-z,\ x\right]$	[2,91]
3	$\left[x,\ z,\ \frac{1}{2}-x\right]$	[3,93]
4	$\left[z,\ x,\ \frac{1}{2}-x\right]$	[4,92]
5	$\left[\frac{1}{2}-z,\ x,\ x\right]$	[5,94]
6	$\left[\frac{1}{2}-x,\ x,\ z\right]$	[6,80]
7	$\left[x,\ \frac{1}{2}-x,\ z\right]$	[7,81]
8	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[8,78]
9	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}-z\right]$	[9,79]
10	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ z\right]$	[10,83]
11	$\left[x,\ x,\ \frac{1}{2}-z\right]$	[11,82]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[12,73]
13	$\left[\frac{1}{2}-x,\ z,\ x\right]$	[13,95]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[14,90]
15	$\left[z,\ \frac{1}{2}-x,\ x\right]$	[15,96]

continued ...

Table 11

No.	position	mapping
16	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[16,89]
17	$[z,\ x,\ x]$	[17,88]
18	$[x,\ z,\ x]$	[18,86]
19	$\left[\frac{1}{2}-x,\ z,\ \frac{1}{2}-x\right]$	[19,74]
20	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ x\right]$	[20,76]
21	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ x\right]$	[21,75]
22	$\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[22,77]
23	$\left[x,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[23,85]
24	$\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-x\right]$	[24,87]
25	$[-x,\ -x,\ -z]$	[25,60]
26	$\left[-x,\ z+\frac{1}{2},\ -x\right]$	[26,67]
27	$\left[-x,\ -z,\ x+\frac{1}{2}\right]$	[27,69]
28	$\left[-z,\ -x,\ x+\frac{1}{2}\right]$	[28,68]
29	$\left[z+\frac{1}{2},\ -x,\ -x\right]$	[29,70]
30	$\left[x+\frac{1}{2},\ -x,\ -z\right]$	[30,56]
31	$\left[-x,\ x+\frac{1}{2},\ -z\right]$	[31,57]
32	$\left[-x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32,54]
33	$\left[x+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	[33,55]
34	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[34,59]
35	$\left[-x,\ -x,\ z+\frac{1}{2}\right]$	[35,58]
36	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[36,49]
37	$\left[x+\frac{1}{2},\ -z,\ -x\right]$	[37,71]
38	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[38,66]
39	$\left[-z,\ x+\frac{1}{2},\ -x\right]$	[39,72]
40	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[40,65]
41	$[-z,\ -x,\ -x]$	[41,64]
42	$[-x,\ -z,\ -x]$	[42,62]
43	$\left[x+\frac{1}{2},\ -z,\ x+\frac{1}{2}\right]$	[43,50]
44	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ -x\right]$	[44,52]
45	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ -x\right]$	[45,51]
46	$\left[-z,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[46,53]
47	$\left[-x,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[47,61]
48	$\left[z+\frac{1}{2},\ -x,\ x+\frac{1}{2}\right]$	[48,63]

Table 12: Wyckoff site: 96l, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x,\ \frac{1}{2}-z,\ y\right]$	[2]
3	$\left[x,\ z,\ \frac{1}{2}-y\right]$	[3]
4	$\left[z,\ y,\ \frac{1}{2}-x\right]$	[4]
5	$\left[\frac{1}{2}-z,\ y,\ x\right]$	[5]
6	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[6]
7	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[7]

continued ...

Table 12

No.	position	mapping
8	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[8]
9	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[9]
10	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[10]
11	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[12]
13	$\left[\frac{1}{2}-x,\ z,\ y\right]$	[13]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[14]
15	$\left[z,\ \frac{1}{2}-y,\ x\right]$	[15]
16	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[16]
17	$[z,\ x,\ y]$	[17]
18	$[y,\ z,\ x]$	[18]
19	$\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}-x\right]$	[19]
20	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y\right]$	[20]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x\right]$	[21]
22	$\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[22]
23	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[23]
24	$\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-y\right]$	[24]
25	$[-x,\ -y,\ -z]$	[25]
26	$\left[-x,\ z+\frac{1}{2},\ -y\right]$	[26]
27	$\left[-x,\ -z,\ y+\frac{1}{2}\right]$	[27]
28	$\left[-z,\ -y,\ x+\frac{1}{2}\right]$	[28]
29	$\left[z+\frac{1}{2},\ -y,\ -x\right]$	[29]
30	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[30]
31	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[31]
32	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32]
33	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[33]
34	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[34]
35	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[35]
36	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[36]
37	$\left[x+\frac{1}{2},\ -z,\ -y\right]$	[37]
38	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[38]
39	$\left[-z,\ y+\frac{1}{2},\ -x\right]$	[39]
40	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[40]
41	$[-z,\ -x,\ -y]$	[41]
42	$[-y,\ -z,\ -x]$	[42]
43	$\left[y+\frac{1}{2},\ -z,\ x+\frac{1}{2}\right]$	[43]
44	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ -y\right]$	[44]
45	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ -x\right]$	[45]
46	$\left[-z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[46]
47	$\left[-y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[47]
48	$\left[z+\frac{1}{2},\ -x,\ y+\frac{1}{2}\right]$	[48]
49	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[49]
50	$\left[x+\frac{1}{2},\ -z,\ y+\frac{1}{2}\right]$	[50]
51	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ -y\right]$	[51]
52	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ -x\right]$	[52]
53	$\left[-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[53]
54	$\left[-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[54]

continued ...

Table 12

No.	position	mapping
55	$\left[y+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	[55]
56	$\left[x+\frac{1}{2},\ -y,\ -z\right]$	[56]
57	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[57]
58	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	[58]
59	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[59]
60	$[-y,\ -x,\ -z]$	[60]
61	$\left[-x,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[61]
62	$[-x,\ -z,\ -y]$	[62]
63	$\left[z+\frac{1}{2},\ -y,\ x+\frac{1}{2}\right]$	[63]
64	$[-z,\ -y,\ -x]$	[64]
65	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[65]
66	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[66]
67	$\left[-y,\ z+\frac{1}{2},\ -x\right]$	[67]
68	$\left[-z,\ -x,\ y+\frac{1}{2}\right]$	[68]
69	$\left[-y,\ -z,\ x+\frac{1}{2}\right]$	[69]
70	$\left[z+\frac{1}{2},\ -x,\ -y\right]$	[70]
71	$\left[y+\frac{1}{2},\ -z,\ -x\right]$	[71]
72	$\left[-z,\ x+\frac{1}{2},\ -y\right]$	[72]
73	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[73]
74	$\left[\frac{1}{2}-x,\ z,\ \frac{1}{2}-y\right]$	[74]
75	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y\right]$	[75]
76	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x\right]$	[76]
77	$\left[z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[77]
78	$\left[y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[78]
79	$\left[\frac{1}{2}-y,\ x,\ \frac{1}{2}-z\right]$	[79]
80	$\left[\frac{1}{2}-x,\ y,\ z\right]$	[80]
81	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[81]
82	$\left[x,\ y,\ \frac{1}{2}-z\right]$	[82]
83	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[83]
84	$[y,\ x,\ z]$	[84]
85	$\left[x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[85]
86	$[x,\ z,\ y]$	[86]
87	$\left[\frac{1}{2}-z,\ y,\ \frac{1}{2}-x\right]$	[87]
88	$[z,\ y,\ x]$	[88]
89	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[89]
90	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[90]
91	$\left[y,\ \frac{1}{2}-z,\ x\right]$	[91]
92	$\left[z,\ x,\ \frac{1}{2}-y\right]$	[92]
93	$\left[y,\ z,\ \frac{1}{2}-x\right]$	[93]
94	$\left[\frac{1}{2}-z,\ x,\ y\right]$	[94]
95	$\left[\frac{1}{2}-y,\ z,\ x\right]$	[95]
96	$\left[z,\ \frac{1}{2}-x,\ y\right]$	[96]