MSG No. 224.115 $P_In\bar{3}m$ [Type IV, cubic]

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[1,8,13,14,74,75,81,82]
2	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[2,3,9,10,73,80,85,86]
3	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[4,16,18,21,77,87,91,95]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[5,15,19,23,76,88,90,93]
5	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[6,11,20,22,79,84,89,96]
6	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[7,12,17,24,78,83,92,94]
7	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[25,32,37,38,50,51,57,58]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[26,27,33,34,49,56,61,62]
9	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[28,40,42,45,53,63,67,71]
10	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[29,39,43,47,52,64,66,69]
11	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[30,35,44,46,55,60,65,72]
12	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[31,36,41,48,54,59,68,70]

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

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

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

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

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	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,3,85,86]`
3	$\left[\frac{3}{4},\ \frac{1}{4},\ -x\right]$	`[4,16,77,87]`
4	$\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{1}{2}\right]$	`[5,15,76,88]`
5	$\left[\frac{1}{4},\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[6,11,79,84]`
6	$\left[\frac{1}{4},\ -x,\ \frac{3}{4}\right]$	`[7,12,78,83]`
7	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[9,10,73,80]`
8	$\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[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	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[26,27,61,62]`
15	$\left[\frac{1}{4},\ \frac{3}{4},\ x\right]$	`[28,40,53,63]`
16	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-x\right]$	`[29,39,52,64]`
17	$\left[\frac{3}{4},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[30,35,55,60]`
18	$\left[\frac{3}{4},\ x,\ \frac{1}{4}\right]$	`[31,36,54,59]`
19	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[33,34,49,56]`
20	$\left[x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[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'.2'm`

No.	position	mapping
1	$\left[\frac{3}{4},\ y,\ y\right]$	`[1,38,61,80]`
2	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	`[2,33,58,75]`
3	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -y\right]$	`[3,34,57,74]`
4	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	`[4,45,66,88]`
5	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	`[5,47,67,87]`
6	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	`[6,46,68,83]`
7	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	`[7,48,65,84]`
8	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{2}-y\right]$	`[8,37,62,73]`
9	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[9,26,51,82]`
10	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y\right]$	`[10,27,50,81]`
11	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	`[11,44,70,78]`
12	$\left[-y,\ \frac{1}{4},\ -y\right]$	`[12,41,72,79]`
13	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[13,32,49,86]`
14	$\left[\frac{1}{4},\ -y,\ -y\right]$	`[14,25,56,85]`
15	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	`[15,43,71,77]`

continued ...

Table 8

No.	position	mapping
16	$\left[-y,\ -y,\ \frac{1}{4}\right]$	[16,42,69,76]
17	$\left[y,\ \frac{3}{4},\ y\right]$	[17,36,55,96]
18	$\left[y,\ y,\ \frac{3}{4}\right]$	[18,40,52,93]
19	$\left[\frac{1}{2}-y,\ y,\ \frac{3}{4}\right]$	[19,39,53,95]
20	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[20,35,54,94]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[21,28,64,90]
22	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[22,30,59,92]
23	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[23,29,63,91]
24	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[24,31,60,89]

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

No.	position	mapping
1	$[0,\ y,\ -y]$	[1,14]
2	$\left[\frac{1}{2},\ y,\ y+\frac{1}{2}\right]$	[2,9]
3	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -y\right]$	[3,10]
4	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ 0\right]$	[4,21]
5	$\left[y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[5,23]
6	$\left[-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[6,22]
7	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	[7,24]
8	$\left[0,\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[8,13]
9	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y\right]$	[11,20]
10	$[-y,\ 0,\ y]$	[12,17]
11	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{2}\right]$	[15,19]
12	$[y,\ -y,\ 0]$	[16,18]
13	$[0,\ -y,\ y]$	[25,38]
14	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-y\right]$	[26,33]
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y\right]$	[27,34]
16	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[28,45]
17	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[29,47]
18	$\left[y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[30,46]
19	$\left[\frac{1}{2}-y,\ 0,\ y+\frac{1}{2}\right]$	[31,48]
20	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[32,37]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ -y\right]$	[35,44]
22	$[y,\ 0,\ -y]$	[36,41]
23	$\left[y+\frac{1}{2},\ y,\ \frac{1}{2}\right]$	[39,43]
24	$[-y,\ y,\ 0]$	[40,42]
25	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[49,62]
26	$\left[0,\ y+\frac{1}{2},\ y\right]$	[50,57]
27	$\left[0,\ -y,\ \frac{1}{2}-y\right]$	[51,58]
28	$\left[-y,\ y,\ \frac{1}{2}\right]$	[52,69]
29	$\left[y+\frac{1}{2},\ y,\ 0\right]$	[53,71]
30	$\left[\frac{1}{2}-y,\ 0,\ -y\right]$	[54,70]
31	$\left[y,\ \frac{1}{2},\ -y\right]$	[55,72]

continued ...

Table 9

No.	position	mapping
32	$\left[\frac{1}{2}, -y, y\right]$	[56,61]
33	$\left[y, 0, y+\frac{1}{2}\right]$	[59,68]
34	$\left[\frac{1}{2}-y, \frac{1}{2}, y+\frac{1}{2}\right]$	[60,65]
35	$\left[-y, \frac{1}{2}-y, 0\right]$	[63,67]
36	$\left[y+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}\right]$	[64,66]
37	$\left[\frac{1}{2}, \frac{1}{2}-y, y+\frac{1}{2}\right]$	[73,86]
38	$\left[0, \frac{1}{2}-y, -y\right]$	[74,81]
39	$\left[0, y, y+\frac{1}{2}\right]$	[75,82]
40	$\left[y, -y, \frac{1}{2}\right]$	[76,93]
41	$\left[\frac{1}{2}-y, -y, 0\right]$	[77,95]
42	$\left[y+\frac{1}{2}, 0, y\right]$	[78,94]
43	$\left[-y, \frac{1}{2}, y\right]$	[79,96]
44	$\left[\frac{1}{2}, y, -y\right]$	[80,85]
45	$\left[-y, 0, \frac{1}{2}-y\right]$	[83,92]
46	$\left[y+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-y\right]$	[84,89]
47	$\left[y, y+\frac{1}{2}, 0\right]$	[87,91]
48	$\left[\frac{1}{2}-y, y+\frac{1}{2}, \frac{1}{2}\right]$	[88,90]

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

No.	position	mapping
1	$\left[\frac{3}{4}, y, z\right]$	[1,80]
2	$\left[\frac{1}{4}, -z, y+\frac{1}{2}\right]$	[2,75]
3	$\left[\frac{1}{4}, z+\frac{1}{2}, -y\right]$	[3,74]
4	$\left[z+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{4}\right]$	[4,88]
5	$\left[-z, y+\frac{1}{2}, \frac{1}{4}\right]$	[5,87]
6	$\left[-y, \frac{1}{4}, z+\frac{1}{2}\right]$	[6,83]
7	$\left[y+\frac{1}{2}, \frac{1}{4}, z+\frac{1}{2}\right]$	[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	$\left[y+\frac{1}{2}, \frac{1}{4}, -z\right]$	[11,78]
12	$\left[-y, \frac{1}{4}, -z\right]$	[12,79]
13	$\left[\frac{1}{4}, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[13,86]
14	$\left[\frac{1}{4}, -z, -y\right]$	[14,85]
15	$\left[z+\frac{1}{2}, -y, \frac{1}{4}\right]$	[15,77]
16	$\left[-z, -y, \frac{1}{4}\right]$	[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	$\left[\frac{3}{4},\ z,\ \frac{1}{2}-y\right]$	[26,51]
27	$\left[\frac{3}{4},\ \frac{1}{2}-z,\ y\right]$	[27,50]
28	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[28,64]
29	$\left[z,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[29,63]
30	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[30,59]
31	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ z\right]$	[35,54]
36	$\left[y,\ \frac{3}{4},\ z\right]$	[36,55]
37	$\left[\frac{3}{4},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[37,62]
38	$\left[\frac{3}{4},\ z,\ y\right]$	[38,61]
39	$\left[\frac{1}{2}-z,\ y,\ \frac{3}{4}\right]$	[39,53]
40	$\left[z,\ y,\ \frac{3}{4}\right]$	[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	$[x,\ x,\ z]$	[1,36]
2	$\left[x+\frac{1}{2},\ -z,\ x+\frac{1}{2}\right]$	[2,43]
3	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ -x\right]$	[3,45]
4	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ -x\right]$	[4,44]
5	$\left[-z,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[5,46]
6	$\left[-x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[6,32]
7	$\left[x+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	[7,33]
8	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[8,30]
9	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}-z\right]$	[9,31]
10	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ z\right]$	[10,35]
11	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[11,34]
12	$[-x,\ -x,\ -z]$	[12,25]
13	$\left[-x,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[13,47]
14	$[-x,\ -z,\ -x]$	[14,42]
15	$\left[z+\frac{1}{2},\ -x,\ x+\frac{1}{2}\right]$	[15,48]

continued ...

Table 11

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

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[x+\frac{1}{2},\ -z,\ y+\frac{1}{2}]$	[2]
3	$[x+\frac{1}{2},\ z+\frac{1}{2},\ -y]$	[3]
4	$[z+\frac{1}{2},\ y+\frac{1}{2},\ -x]$	[4]
5	$[-z,\ y+\frac{1}{2},\ x+\frac{1}{2}]$	[5]
6	$[-y,\ x+\frac{1}{2},\ z+\frac{1}{2}]$	[6]
7	$[y+\frac{1}{2},\ -x,\ z+\frac{1}{2}]$	[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	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[11]
12	$[-y,\ -x,\ -z]$	[12]
13	$\left[-x,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[13]
14	$[-x,\ -z,\ -y]$	[14]
15	$\left[z+\frac{1}{2},\ -y,\ x+\frac{1}{2}\right]$	[15]
16	$[-z,\ -y,\ -x]$	[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	$\left[\frac{1}{2}-x,\ z,\ \frac{1}{2}-y\right]$	[26]
27	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y\right]$	[27]
28	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x\right]$	[28]
29	$\left[z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[29]
30	$\left[y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\ x,\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[35]
36	$[y,\ x,\ z]$	[36]
37	$\left[x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[37]
38	$[x,\ z,\ y]$	[38]
39	$\left[\frac{1}{2}-z,\ y,\ \frac{1}{2}-x\right]$	[39]
40	$[z,\ y,\ x]$	[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	$\left[x,\ \frac{1}{2}-z,\ y\right]$	[50]
51	$\left[x,\ z,\ \frac{1}{2}-y\right]$	[51]
52	$\left[z,\ y,\ \frac{1}{2}-x\right]$	[52]
53	$\left[\frac{1}{2}-z,\ y,\ x\right]$	[53]
54	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[54]

continued ...

Table 12

No.	position	mapping
55	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[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	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[59]
60	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[60]
61	$\left[\frac{1}{2}-x,\ z,\ y\right]$	[61]
62	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[62]
63	$\left[z,\ \frac{1}{2}-y,\ x\right]$	[63]
64	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[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	$\left[-x,\ z+\frac{1}{2},\ -y\right]$	[74]
75	$\left[-x,\ -z,\ y+\frac{1}{2}\right]$	[75]
76	$\left[-z,\ -y,\ x+\frac{1}{2}\right]$	[76]
77	$\left[z+\frac{1}{2},\ -y,\ -x\right]$	[77]
78	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[78]
79	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[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	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[83]
84	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[84]
85	$\left[x+\frac{1}{2},\ -z,\ -y\right]$	[85]
86	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[86]
87	$\left[-z,\ y+\frac{1}{2},\ -x\right]$	[87]
88	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[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]