MSG No. 229.142 $Im'\bar{3}'m$ [Type III, cubic]

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[1,2,39,40,61,62,81,82]
2	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[3,4,37,38,69,70,73,74]
3	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[5,12,44,46,65,67,78,80]
4	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[6,9,43,47,64,71,75,84]
5	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[7,11,42,45,63,72,76,83]
6	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[8,10,41,48,66,68,77,79]
7	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[13,14,33,34,49,50,87,88]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[15,24,28,35,55,59,90,93]
9	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[16,23,27,36,54,57,91,95]
10	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[17,19,30,32,53,60,92,94]
11	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[18,20,29,31,56,58,89,96]
12	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[21,22,25,26,51,52,85,86]

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ y]$	`[1,22,33,38]`
2	$[0,\ -y,\ -y]$	`[2,21,34,37]`
3	$[0,\ y,\ -y]$	`[3,13,26,40]`
4	$[0,\ -y,\ y]$	`[4,14,25,39]`
5	$[y,\ 0,\ y]$	`[5,20,30,48]`
6	$[y,\ y,\ 0]$	`[6,24,27,45]`
7	$[-y,\ y,\ 0]$	`[7,23,28,47]`
8	$[-y,\ 0,\ y]$	`[8,19,29,46]`
9	$[-y,\ -y,\ 0]$	`[9,15,36,42]`
10	$[y,\ 0,\ -y]$	`[10,17,31,44]`
11	$[y,\ -y,\ 0]$	`[11,16,35,43]`
12	$[-y,\ 0,\ -y]$	`[12,18,32,41]`
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[49,70,81,86]`
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-y\right]$	`[50,69,82,85]`
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[51,61,74,88]`

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[52,62,73,87]
17	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[53,68,78,96]
18	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[54,72,75,93]
19	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[55,71,76,95]
20	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[56,67,77,94]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[57,63,84,90]
22	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[58,65,79,92]
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[59,64,83,91]
24	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[60,66,80,89]

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

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	[1,82]
2	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	[2,81]
3	$\left[\frac{3}{4},\ y,\ y+\frac{1}{2}\right]$	[3,73]
4	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}-y\right]$	[4,74]
5	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	[5,80]
6	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[6,84]
7	$\left[-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[7,83]
8	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y\right]$	[8,79]
9	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[9,75]
10	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ -y\right]$	[10,77]
11	$\left[y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[11,76]
12	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[12,78]
13	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ -y\right]$	[13,87]
14	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y\right]$	[14,88]
15	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	[15,93]
16	$\left[\frac{1}{2}-y,\ -y,\ \frac{3}{4}\right]$	[16,95]
17	$\left[y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[17,94]
18	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[18,96]
19	$\left[-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[19,92]
20	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[20,89]
21	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -y\right]$	[21,86]
22	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	[22,85]
23	$\left[y+\frac{1}{2},\ y,\ \frac{3}{4}\right]$	[23,91]
24	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{4}\right]$	[24,90]
25	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y\right]$	[25,51]
26	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ -y\right]$	[26,52]
27	$\left[\frac{1}{2}-y,\ y,\ \frac{3}{4}\right]$	[27,57]
28	$\left[y+\frac{1}{2},\ y,\ \frac{1}{4}\right]$	[28,59]
29	$\left[-y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[29,58]
30	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[30,60]
31	$\left[y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[31,56]

continued ...

Table 9

No.	position	mapping
32	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[32,53]
33	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y\right]$	[33,50]
34	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -y\right]$	[34,49]
35	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{4}\right]$	[35,55]
36	$\left[y+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[36,54]
37	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	[37,70]
38	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	[38,69]
39	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-y\right]$	[39,61]
40	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	[40,62]
41	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[41,68]
42	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[42,72]
43	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[43,71]
44	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ -y\right]$	[44,67]
45	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[45,63]
46	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y\right]$	[46,65]
47	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[47,64]
48	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[48,66]

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

No.	position	mapping
1	$[0,\ y,\ z]$	[1,38]
2	$[0,\ -y,\ -z]$	[2,37]
3	$[0,\ y,\ -z]$	[3,40]
4	$[0,\ -y,\ z]$	[4,39]
5	$[z,\ 0,\ y]$	[5,48]
6	$[y,\ z,\ 0]$	[6,45]
7	$[-y,\ z,\ 0]$	[7,47]
8	$[-z,\ 0,\ y]$	[8,46]
9	$[-y,\ -z,\ 0]$	[9,42]
10	$[z,\ 0,\ -y]$	[10,44]
11	$[y,\ -z,\ 0]$	[11,43]
12	$[-z,\ 0,\ -y]$	[12,41]
13	$[0,\ z,\ -y]$	[13,26]
14	$[0,\ -z,\ y]$	[14,25]
15	$[-z,\ -y,\ 0]$	[15,36]
16	$[z,\ -y,\ 0]$	[16,35]
17	$[y,\ 0,\ -z]$	[17,31]
18	$[-y,\ 0,\ -z]$	[18,32]
19	$[-y,\ 0,\ z]$	[19,29]
20	$[y,\ 0,\ z]$	[20,30]
21	$[0,\ -z,\ -y]$	[21,34]
22	$[0,\ z,\ y]$	[22,33]
23	$[-z,\ y,\ 0]$	[23,28]

continued ...

Table 10

No.	position	mapping
24	$[z,\ y,\ 0]$	[24,27]
25	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[49,86]
26	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[50,85]
27	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[51,88]
28	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[52,87]
29	$\left[z+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[53,96]
30	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[54,93]
31	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[55,95]
32	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[56,94]
33	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[57,90]
34	$\left[z+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[58,92]
35	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[59,91]
36	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[60,89]
37	$\left[\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[61,74]
38	$\left[\frac{1}{2},\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[62,73]
39	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[63,84]
40	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[64,83]
41	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[65,79]
42	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[66,80]
43	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[67,77]
44	$\left[y+\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[68,78]
45	$\left[\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[69,82]
46	$\left[\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[70,81]
47	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[71,76]
48	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[72,75]

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

No.	position	mapping
1	$[x,\ x,\ z]$	[1,20]
2	$[x,\ -x,\ -z]$	[2,17]
3	$[-x,\ x,\ -z]$	[3,18]
4	$[-x,\ -x,\ z]$	[4,19]
5	$[z,\ x,\ x]$	[5,24]
6	$[x,\ z,\ x]$	[6,22]
7	$[-x,\ z,\ -x]$	[7,13]
8	$[-z,\ -x,\ x]$	[8,15]
9	$[-x,\ -z,\ x]$	[9,14]
10	$[z,\ -x,\ -x]$	[10,16]
11	$[x,\ -z,\ -x]$	[11,21]
12	$[-z,\ x,\ -x]$	[12,23]
13	$[x,\ -z,\ x]$	[25,43]
14	$[x,\ z,\ -x]$	[26,45]
15	$[z,\ x,\ -x]$	[27,44]

continued ...

Table 11

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

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

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

continued ...

Table 12

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

continued ...

Table 12

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