MSG No. 229.144 $Im'\bar{3}'m'$ [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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,8,9,10,13,14,25,26,27,32,33,34,37,38]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4,5,15,16,18,19,21,23,28,29,39,40,42,43,45,47]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[6,7,11,12,17,20,22,24,30,31,35,36,41,44,46,48]
4	$\left[\frac{1}{2}, 0, 0\right]$	[49,50,51,56,57,58,61,62,73,74,75,80,81,82,85,86]
5	$\left[0, 0, \frac{1}{2}\right]$	[52,53,63,64,66,67,69,71,76,77,87,88,90,91,93,95]
6	$\left[0, \frac{1}{2}, 0\right]$	[54,55,59,60,65,68,70,72,78,79,83,84,89,92,94,96]

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[1,8,33,34,61,62,74,75]
2	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[2,3,37,38,57,58,73,80]
3	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[4,16,29,39,66,69,91,95]
4	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[5,15,28,40,67,71,90,93]
5	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[6,11,31,36,68,70,89,96]
6	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[7,12,30,35,65,72,92,94]
7	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[9,10,25,32,50,51,85,86]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[13,14,26,27,49,56,81,82]
9	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[17,24,44,46,55,60,78,83]
10	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[18,21,43,47,52,64,77,87]
11	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[19,23,42,45,53,63,76,88]
12	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[20,22,41,48,54,59,79,84]

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ y]$	`[1,13,32,38]`
2	$[0,\ -y,\ y]$	`[2,10,27,33]`
3	$[0,\ y,\ -y]$	`[3,9,26,34]`
4	$[y,\ y,\ 0]$	`[4,18,40,45]`
5	$[-y,\ y,\ 0]$	`[5,19,39,47]`
6	$[-y,\ 0,\ y]$	`[6,20,35,46]`
7	$[y,\ 0,\ y]$	`[7,17,36,48]`
8	$[0,\ -y,\ -y]$	`[8,14,25,37]`
9	$[y,\ 0,\ -y]$	`[11,22,30,44]`
10	$[-y,\ 0,\ -y]$	`[12,24,31,41]`
11	$[y,\ -y,\ 0]$	`[15,23,29,43]`
12	$[-y,\ -y,\ 0]$	`[16,21,28,42]`
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[49,61,80,86]`
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	`[50,58,75,81]`
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[51,57,74,82]`

continued ...

Table 8

No.	position	mapping
16	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	[52,66,88,93]
17	$\left[\frac{1}{2}-y, y+\frac{1}{2}, \frac{1}{2}\right]$	[53,67,87,95]
18	$\left[\frac{1}{2}-y, \frac{1}{2}, y+\frac{1}{2}\right]$	[54,68,83,94]
19	$\left[y+\frac{1}{2}, \frac{1}{2}, y+\frac{1}{2}\right]$	[55,65,84,96]
20	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-y\right]$	[56,62,73,85]
21	$\left[y+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-y\right]$	[59,70,78,92]
22	$\left[\frac{1}{2}-y, \frac{1}{2}, \frac{1}{2}-y\right]$	[60,72,79,89]
23	$\left[y+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}\right]$	[63,71,77,91]
24	$\left[\frac{1}{2}-y, \frac{1}{2}-y, \frac{1}{2}\right]$	[64,69,76,90]

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

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

continued ...

Table 9

No.	position	mapping
32	$\left[\frac{3}{4}, y, \frac{1}{2}-y\right]$	[32,85]
33	$\left[\frac{1}{4}, -y, \frac{1}{2}-y\right]$	[33,74]
34	$\left[\frac{1}{4}, y, y+\frac{1}{2}\right]$	[34,75]
35	$\left[-y, \frac{3}{4}, \frac{1}{2}-y\right]$	[35,92]
36	$\left[y, \frac{1}{4}, \frac{1}{2}-y\right]$	[36,89]
37	$\left[\frac{1}{4}, y+\frac{1}{2}, -y\right]$	[37,80]
38	$\left[\frac{1}{4}, \frac{1}{2}-y, y\right]$	[38,73]
39	$\left[y+\frac{1}{2}, y, \frac{3}{4}\right]$	[39,91]
40	$\left[\frac{1}{2}-y, y, \frac{1}{4}\right]$	[40,90]
41	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[41,84]
42	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[42,88]
43	$\left[y, y+\frac{1}{2}, \frac{1}{4}\right]$	[43,87]
44	$\left[\frac{1}{2}-y, \frac{1}{4}, -y\right]$	[44,83]
45	$\left[y, \frac{1}{2}-y, \frac{3}{4}\right]$	[45,76]
46	$\left[y+\frac{1}{2}, \frac{1}{4}, y\right]$	[46,78]
47	$\left[-y, \frac{1}{2}-y, \frac{1}{4}\right]$	[47,77]
48	$\left[\frac{1}{2}-y, \frac{3}{4}, y\right]$	[48,79]

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

No.	position	mapping
1	$[0, y, z]$	[1,32]
2	$[0, -z, y]$	[2,27]
3	$[0, z, -y]$	[3,26]
4	$[z, y, 0]$	[4,40]
5	$[-z, y, 0]$	[5,39]
6	$[-y, 0, z]$	[6,35]
7	$[y, 0, z]$	[7,36]
8	$[0, -y, -z]$	[8,25]
9	$[0, y, -z]$	[9,34]
10	$[0, -y, z]$	[10,33]
11	$[y, 0, -z]$	[11,30]
12	$[-y, 0, -z]$	[12,31]
13	$[0, z, y]$	[13,38]
14	$[0, -z, -y]$	[14,37]
15	$[z, -y, 0]$	[15,29]
16	$[-z, -y, 0]$	[16,28]
17	$[z, 0, y]$	[17,48]
18	$[y, z, 0]$	[18,45]
19	$[-y, z, 0]$	[19,47]
20	$[-z, 0, y]$	[20,46]
21	$[-y, -z, 0]$	[21,42]
22	$[z, 0, -y]$	[22,44]
23	$[y, -z, 0]$	[23,43]

continued ...

Table 10

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

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

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

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

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

continued ...

Table 12

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

continued ...

Table 12

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