MSG No. 229.143 $Im\bar{3}m'$ [Type III, cubic]

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

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'/mm.m'

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[1,2,15,16,81,82,85,86]
2	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[3,4,13,14,73,74,93,94]
3	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[5,12,20,22,78,80,89,91]
4	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[6,9,19,23,75,84,88,95]
5	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[7,11,18,21,76,83,87,96]
6	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[8,10,17,24,77,79,90,92]
7	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[25,26,45,46,51,52,61,62]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[27,36,40,47,54,57,67,71]
9	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[28,35,39,48,55,59,66,69]
10	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[29,31,42,44,56,58,65,72]
11	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[30,32,41,43,53,60,68,70]
12	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[33,34,37,38,49,50,63,64]

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ y]$	`[1,14,33,46]`
2	$[0,\ -y,\ -y]$	`[2,13,34,45]`
3	$[0,\ y,\ -y]$	`[3,16,26,37]`
4	$[0,\ -y,\ y]$	`[4,15,25,38]`
5	$[y,\ 0,\ y]$	`[5,24,30,44]`
6	$[y,\ y,\ 0]$	`[6,21,27,48]`
7	$[-y,\ y,\ 0]$	`[7,23,28,47]`
8	$[-y,\ 0,\ y]$	`[8,22,29,43]`
9	$[-y,\ -y,\ 0]$	`[9,18,36,39]`
10	$[y,\ 0,\ -y]$	`[10,20,31,41]`
11	$[y,\ -y,\ 0]$	`[11,19,35,40]`
12	$[-y,\ 0,\ -y]$	`[12,17,32,42]`
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[49,62,81,94]`
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-y\right]$	`[50,61,82,93]`
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[51,64,74,85]`

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[52,63,73,86]
17	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[53,72,78,92]
18	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[54,69,75,96]
19	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[55,71,76,95]
20	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[56,70,77,91]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[57,66,84,87]
22	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[58,68,79,89]
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[59,67,83,88]
24	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[60,65,80,90]

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	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	[13,94]
14	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	[14,93]
15	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-y\right]$	[15,85]
16	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	[16,86]
17	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[17,92]
18	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[18,96]
19	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[19,95]
20	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ -y\right]$	[20,91]
21	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[21,87]
22	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y\right]$	[22,89]
23	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[23,88]
24	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[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	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ -y\right]$	[37,63]
38	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y\right]$	[38,64]
39	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	[39,69]
40	$\left[\frac{1}{2}-y,\ -y,\ \frac{3}{4}\right]$	[40,71]
41	$\left[y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[41,70]
42	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[42,72]
43	$\left[-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[43,68]
44	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[44,65]
45	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -y\right]$	[45,62]
46	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	[46,61]
47	$\left[y+\frac{1}{2},\ y,\ \frac{3}{4}\right]$	[47,67]
48	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{4}\right]$	[48,66]

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

No.	position	mapping
1	$[0,\ y,\ z]$	[1,14]
2	$[0,\ -y,\ -z]$	[2,13]
3	$[0,\ y,\ -z]$	[3,16]
4	$[0,\ -y,\ z]$	[4,15]
5	$[z,\ 0,\ y]$	[5,24]
6	$[y,\ z,\ 0]$	[6,21]
7	$[-y,\ z,\ 0]$	[7,23]
8	$[-z,\ 0,\ y]$	[8,22]
9	$[-y,\ -z,\ 0]$	[9,18]
10	$[z,\ 0,\ -y]$	[10,20]
11	$[y,\ -z,\ 0]$	[11,19]
12	$[-z,\ 0,\ -y]$	[12,17]
13	$[0,\ -z,\ y]$	[25,38]
14	$[0,\ z,\ -y]$	[26,37]
15	$[z,\ y,\ 0]$	[27,48]
16	$[-z,\ y,\ 0]$	[28,47]
17	$[-y,\ 0,\ z]$	[29,43]
18	$[y,\ 0,\ z]$	[30,44]
19	$[y,\ 0,\ -z]$	[31,41]
20	$[-y,\ 0,\ -z]$	[32,42]
21	$[0,\ z,\ y]$	[33,46]
22	$[0,\ -z,\ -y]$	[34,45]
23	$[z,\ -y,\ 0]$	[35,40]

continued ...

Table 10

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

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

No.	position	mapping
1	$[x,\ x,\ z]$	[1,44]
2	$[x,\ -x,\ -z]$	[2,41]
3	$[-x,\ x,\ -z]$	[3,42]
4	$[-x,\ -x,\ z]$	[4,43]
5	$[z,\ x,\ x]$	[5,48]
6	$[x,\ z,\ x]$	[6,46]
7	$[-x,\ z,\ -x]$	[7,37]
8	$[-z,\ -x,\ x]$	[8,39]
9	$[-x,\ -z,\ x]$	[9,38]
10	$[z,\ -x,\ -x]$	[10,40]
11	$[x,\ -z,\ -x]$	[11,45]
12	$[-z,\ x,\ -x]$	[12,47]
13	$[-x,\ -x,\ -z]$	[13,32]
14	$[-x,\ x,\ z]$	[14,29]
15	$[x,\ -x,\ z]$	[15,30]

continued ...

Table 11

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

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	$[-x, -y, -z]$	[13]
14	$[-x, y, z]$	[14]
15	$[x, -y, z]$	[15]
16	$[x, y, -z]$	[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	$[x, -z, y]$	[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	$[-x, z, -y]$	[37]
38	$[-x, -z, y]$	[38]
39	$[-z, -y, x]$	[39]
40	$[z, -y, -x]$	[40]
41	$[y, -x, -z]$	[41]
42	$[-y, x, -z]$	[42]
43	$[-y, -x, z]$	[43]
44	$[y, x, z]$	[44]
45	$[x, -z, -y]$	[45]
46	$[x, z, y]$	[46]
47	$[-z, y, -x]$	[47]
48	$[z, y, x]$	[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[61]
62	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[62]
63	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[63]
64	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[64]
65	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[65]
66	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[66]
67	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[67]
68	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[68]
69	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[69]
70	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[70]
71	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[71]
72	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[85]
86	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[86]
87	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x+\frac{1}{2}\right]$	[87]
88	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[88]
89	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[89]
90	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[90]
91	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[91]
92	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[92]
93	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[93]
94	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[94]
95	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	[95]
96	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[96]