MSG No. 224.111 $Pn\bar{3}m1'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: -43m1'

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

Table 2: Wyckoff site: 4b, site symmetry: .-3m1'

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

Table 3: Wyckoff site: 4c, site symmetry: .-3m1'

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

Table 4: Wyckoff site: 6d, site symmetry: -42.m1'

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

Table 5: Wyckoff site: 8e, site symmetry: .3m1'

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

Table 6: Wyckoff site: 12f, site symmetry: 2.221'

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

Table 7: Wyckoff site: 12g, site symmetry: 2.mm1'

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

Table 8: Wyckoff site: `24h`, site symmetry: `2..1'`

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

Table 9: Wyckoff site: `24i`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ y+\frac{1}{2}\right]$	`[1,13,49,61]`
2	$\left[0,\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	`[2,10,50,58]`
3	$[0,\ y,\ -y]$	`[3,9,51,57]`
4	$\left[y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[4,18,52,66]`
5	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ 0\right]$	`[5,19,53,67]`
6	$[-y,\ 0,\ y]$	`[6,20,54,68]`
7	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y\right]$	`[7,17,55,65]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -y\right]$	`[8,14,56,62]`
9	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	`[11,22,59,70]`
10	$\left[-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	`[12,24,60,72]`
11	$[y,\ -y,\ 0]$	`[15,23,63,71]`
12	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{2}\right]$	`[16,21,64,69]`
13	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-y\right]$	`[25,37,73,85]`
14	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[26,34,74,82]`
15	$[0,\ -y,\ y]$	`[27,33,75,81]`

continued ...

Table 9

No.	position	mapping
16	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[28,42,76,90]
17	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[29,43,77,91]
18	$[y,\ 0,\ -y]$	[30,44,78,92]
19	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ -y\right]$	[31,41,79,89]
20	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y\right]$	[32,38,80,86]
21	$\left[\frac{1}{2}-y,\ 0,\ y+\frac{1}{2}\right]$	[35,46,83,94]
22	$\left[y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[36,48,84,96]
23	$[-y,\ y,\ 0]$	[39,47,87,95]
24	$\left[y+\frac{1}{2},\ y,\ \frac{1}{2}\right]$	[40,45,88,93]

Table 10: Wyckoff site: 24j, site symmetry: ..21'

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

Table 11: Wyckoff site: `24k`, site symmetry: `..m1'`

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

Table 12: Wyckoff site: `48l`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,49]`
2	$\left[x+\frac{1}{2},\ -z,\ y+\frac{1}{2}\right]$	`[2,50]`
3	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ -y\right]$	`[3,51]`
4	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ -x\right]$	`[4,52]`
5	$\left[-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[5,53]`
6	$\left[-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[6,54]`
7	$\left[y+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	`[7,55]`
8	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[8,56]`
9	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	`[9,57]`
10	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	`[10,58]`
11	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	`[11,59]`
12	$[-y,\ -x,\ -z]$	`[12,60]`
13	$\left[-x,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[13,61]`
14	$[-x,\ -z,\ -y]$	`[14,62]`
15	$\left[z+\frac{1}{2},\ -y,\ x+\frac{1}{2}\right]$	`[15,63]`

continued ...

Table 12

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