MSG No. 211.57 $I4321'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 4321'

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,
		49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,
		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: 42.21'

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

Table 3: Wyckoff site: 8c, site symmetry: .321'

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

Table 4: Wyckoff site: 12d, site symmetry: 2.221'

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[1,8,37,38,49,56,85,86]
2	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[2,3,33,34,50,51,81,82]
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[4,16,42,45,52,64,90,93]
4	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[5,15,43,47,53,63,91,95]
5	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[6,11,44,46,54,59,92,94]
6	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[7,12,41,48,55,60,89,96]
7	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[9,10,26,27,57,58,74,75]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[13,14,25,32,61,62,73,80]
9	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[17,24,31,36,65,72,79,84]
10	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[18,21,28,40,66,69,76,88]
11	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[19,23,29,39,67,71,77,87]
12	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[20,22,30,35,68,70,78,83]

Table 5: Wyckoff site: 12e, site symmetry: 4..1'

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

Table 6: Wyckoff site: 16f, site symmetry: .3.1'

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

Table 7: Wyckoff site: `24g`, site symmetry: `2..1'`

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

Table 8: Wyckoff site: `24h`, site symmetry: `..21'`

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

continued ...

Table 8

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

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

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

Table 10: Wyckoff site: `48j`, site symmetry: `11'`

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

continued ...

Table 10

No.	position	mapping
47	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[47,95]
48	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[48,96]