MSG No. 223.105 $Pm\bar{3}n1'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: m-3.1'

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

Table 2: Wyckoff site: 6b, site symmetry: mmm..1'

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

Table 3: Wyckoff site: 6c, site symmetry: -4m.21'

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

Table 4: Wyckoff site: 6d, site symmetry: -4m.21'

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

Table 5: Wyckoff site: 8e, site symmetry: .321'

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

Table 6: Wyckoff site: 12f, site symmetry: 2mm..1'

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

Table 7: Wyckoff site: 12g, site symmetry: 2mm..1'

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

Table 8: Wyckoff site: `12h`, site symmetry: `2mm..1'`

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

Table 9: Wyckoff site: `16i`, site symmetry: `.3.1'`

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	`[1,13,49,61]`
2	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	`[2,10,50,58]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,9,51,57]`
4	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	`[4,18,52,66]`
5	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	`[5,19,53,67]`

continued ...

Table 10

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

Table 11: Wyckoff site: 24k, site symmetry: m..1'

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

continued ...

Table 11

No.	position	mapping
22	$[z, 0, -y]$	[22,44,70,92]
23	$[y, -z, 0]$	[23,43,71,91]
24	$[-z, 0, -y]$	[24,41,72,89]

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

No.	position	mapping
1	$[x, y, z]$	[1,49]
2	$\left[x+\frac{1}{2}, \frac{1}{2}-z, y+\frac{1}{2}\right]$	[2,50]
3	$\left[x+\frac{1}{2}, z+\frac{1}{2}, \frac{1}{2}-y\right]$	[3,51]
4	$\left[z+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-x\right]$	[4,52]
5	$\left[\frac{1}{2}-z, y+\frac{1}{2}, x+\frac{1}{2}\right]$	[5,53]
6	$\left[\frac{1}{2}-y, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[6,54]
7	$\left[y+\frac{1}{2}, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[7,55]
8	$[x, -y, -z]$	[8,56]
9	$[-x, y, -z]$	[9,57]
10	$[-x, -y, z]$	[10,58]
11	$\left[y+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[11,59]
12	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[12,60]
13	$\left[\frac{1}{2}-x, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[13,61]
14	$\left[\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[14,62]
15	$\left[z+\frac{1}{2}, \frac{1}{2}-y, x+\frac{1}{2}\right]$	[15,63]
16	$\left[\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[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	$[-x, -y, -z]$	[25,73]
26	$\left[\frac{1}{2}-x, z+\frac{1}{2}, \frac{1}{2}-y\right]$	[26,74]
27	$\left[\frac{1}{2}-x, \frac{1}{2}-z, y+\frac{1}{2}\right]$	[27,75]
28	$\left[\frac{1}{2}-z, \frac{1}{2}-y, x+\frac{1}{2}\right]$	[28,76]
29	$\left[z+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[29,77]
30	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[30,78]
31	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[31,79]
32	$[-x, y, z]$	[32,80]
33	$[x, -y, z]$	[33,81]
34	$[x, y, -z]$	[34,82]
35	$\left[\frac{1}{2}-y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[35,83]
36	$\left[y+\frac{1}{2}, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[36,84]
37	$\left[x+\frac{1}{2}, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[37,85]

continued ...

Table 12

No.	position	mapping
38	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[38,86]
39	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[39,87]
40	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[40,88]
41	$[-z,\, -x,\, -y]$	[41,89]
42	$[-y,\, -z,\, -x]$	[42,90]
43	$[y,\, -z,\, x]$	[43,91]
44	$[z,\, x,\, -y]$	[44,92]
45	$[y,\, z,\, -x]$	[45,93]
46	$[-z,\, x,\, y]$	[46,94]
47	$[-y,\, z,\, x]$	[47,95]
48	$[z,\, -x,\, y]$	[48,96]