MSG No. 200.14 $Pm\bar{3}$ [Type I, cubic]

Table 1: Wyckoff site: `1a`, site symmetry: `m-3.`

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]`

Table 2: Wyckoff site: `1b`, site symmetry: `m-3.`

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]`

Table 3: Wyckoff site: `3c`, site symmetry: `mmm..`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,13,14,15,16]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[5,8,10,12,17,20,22,24]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6,7,9,11,18,19,21,23]`

Table 4: Wyckoff site: `3d`, site symmetry: `mmm..`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	`[1,2,3,4,13,14,15,16]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[5,8,10,12,17,20,22,24]`
3	$\left[0, 0, \frac{1}{2}\right]$	`[6,7,9,11,18,19,21,23]`

Table 5: Wyckoff site: `6e`, site symmetry: `2mm..`

No.	position	mapping
1	$[x, 0, 0]$	`[1,2,15,16]`
2	$[-x, 0, 0]$	`[3,4,13,14]`
3	$[0, x, 0]$	`[5,12,20,22]`
4	$[0, 0, x]$	`[6,9,19,23]`
5	$[0, 0, -x]$	`[7,11,18,21]`
6	$[0, -x, 0]$	`[8,10,17,24]`

Table 6: Wyckoff site: `6f`, 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]`

Table 7: Wyckoff site: `6g`, site symmetry: `2mm..`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,2,15,16]`
2	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[3,4,13,14]`
3	$\left[0,\ x,\ \frac{1}{2}\right]$	`[5,12,20,22]`
4	$\left[\frac{1}{2},\ 0,\ x\right]$	`[6,9,19,23]`
5	$\left[\frac{1}{2},\ 0,\ -x\right]$	`[7,11,18,21]`
6	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[8,10,17,24]`

Table 8: Wyckoff site: `6h`, site symmetry: `2mm..`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[1,2,15,16]`
2	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[3,4,13,14]`
3	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[5,12,20,22]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ x\right]$	`[6,9,19,23]`
5	$\left[\frac{1}{2},\ \frac{1}{2},\ -x\right]$	`[7,11,18,21]`
6	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[8,10,17,24]`

Table 9: Wyckoff site: `8i`, site symmetry: `.3.`

No.	position	mapping
1	$[x,\ x,\ x]$	`[1,5,6]`
2	$[x,\ -x,\ -x]$	`[2,10,11]`
3	$[-x,\ x,\ -x]$	`[3,7,12]`
4	$[-x,\ -x,\ x]$	`[4,8,9]`
5	$[-x,\ -x,\ -x]$	`[13,17,18]`
6	$[-x,\ x,\ x]$	`[14,22,23]`
7	$[x,\ -x,\ x]$	`[15,19,24]`
8	$[x,\ x,\ -x]$	`[16,20,21]`

Table 10: Wyckoff site: `12j`, 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]`

Table 11: Wyckoff site: `12k`, site symmetry: `m..`

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ z\right]$	`[1,14]`
2	$\left[\frac{1}{2},\ -y,\ -z\right]$	`[2,13]`
3	$\left[\frac{1}{2},\ y,\ -z\right]$	`[3,16]`
4	$\left[\frac{1}{2},\ -y,\ z\right]$	`[4,15]`
5	$\left[z,\ \frac{1}{2},\ y\right]$	`[5,24]`
6	$\left[y,\ z,\ \frac{1}{2}\right]$	`[6,21]`
7	$\left[-y,\ z,\ \frac{1}{2}\right]$	`[7,23]`
8	$\left[-z,\ \frac{1}{2},\ y\right]$	`[8,22]`
9	$\left[-y,\ -z,\ \frac{1}{2}\right]$	`[9,18]`
10	$\left[z,\ \frac{1}{2},\ -y\right]$	`[10,20]`
11	$\left[y,\ -z,\ \frac{1}{2}\right]$	`[11,19]`
12	$\left[-z,\ \frac{1}{2},\ -y\right]$	`[12,17]`

Table 12: Wyckoff site: `24l`, 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]`
8	$[-z,\ -x,\ y]$	`[8]`
9	$[-y,\ -z,\ x]$	`[9]`

continued ...

Table 12

No.	position	mapping
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]