MSG No. 201.18 $Pn\bar{3}$ [Type I, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `23.`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `.-3.`

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

Table 4: Wyckoff site: `6d`, site symmetry: `222..`

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

Table 5: Wyckoff site: `8e`, site symmetry: `.3.`

No.	position	mapping
1	$[x, x, x]$	`[1,5,6]`
2	$\left[x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	`[2,10,11]`

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2..

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

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

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

Table 8: Wyckoff site: 24h, site symmetry: 1

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