MSG No. 87.78 $I4/m'$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/m'..`

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

Table 2: Wyckoff site: `2b`, site symmetry: `4/m'..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2/m'..`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4'..`

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

Table 5: Wyckoff site: `4e`, site symmetry: `4..`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,2,3,4]`
2	$[0,\ 0,\ -z]$	`[5,6,7,8]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,10,11,12]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[13,14,15,16]`

Table 6: Wyckoff site: `8f`, site symmetry: `-1'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,13]`
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[2,14]`
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[3,15]`
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,16]`
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[5,9]`
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[6,10]`
7	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[7,11]`
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[8,12]`

Table 7: Wyckoff site: `8g`, site symmetry: `2..`

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	`[1,4]`
2	$\left[\frac{1}{2}, 0, z\right]$	`[2,3]`
3	$\left[0, \frac{1}{2}, -z\right]$	`[5,8]`
4	$\left[\frac{1}{2}, 0, -z\right]$	`[6,7]`
5	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	`[9,12]`
6	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	`[10,11]`
7	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	`[13,16]`
8	$\left[0, \frac{1}{2}, \frac{1}{2}-z\right]$	`[14,15]`

Table 8: Wyckoff site: `8h`, site symmetry: `m'..`

No.	position	mapping
1	$[x, y, 0]$	`[1,8]`
2	$[-y, x, 0]$	`[2,7]`
3	$[y, -x, 0]$	`[3,6]`
4	$[-x, -y, 0]$	`[4,5]`
5	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	`[9,16]`
6	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}\right]$	`[10,15]`
7	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	`[11,14]`
8	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}\right]$	`[12,13]`

Table 9: Wyckoff site: `16i`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$[-y, x, z]$	`[2]`
3	$[y, -x, z]$	`[3]`

continued ...

Table 9

No.	position	mapping
4	$[-x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[y, -x, -z]$	[6]
7	$[-y, x, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[9]
10	$\left[\frac{1}{2}-y, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[10]
11	$\left[y+\frac{1}{2}, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[11]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[12]
13	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[13]
14	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[14]
15	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[15]
16	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[16]