MSG No. 85.66 P_I4/n [Type IV, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$\left[\frac{1}{2}-y, x, z\right]$	`[2]`
3	$\left[y, \frac{1}{2}-x, z\right]$	`[3]`

continued ...

Table 9

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