MSG No. 86.74 P_I4_2/n [Type IV, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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