MSG No. 87.79 $I4'/m'$ [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	$\left[0, \frac{1}{2}, 0\right]$	[1,2,7,8]
2	$\left[\frac{1}{2}, 0, 0\right]$	[3,4,5,6]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[9,10,15,16]
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[11,12,13,14]

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 9

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