MSG No. 87.77 $I4'/m$ [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	$\left[0, \frac{1}{2}, 0\right]$	`[1,2,3,4]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[5,6,7,8]`
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[9,10,11,12]`
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[13,14,15,16]`

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

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

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	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,11]`
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[2,12]`
3	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[3,9]`
4	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[4,10]`
5	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[5,15]`
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[6,16]`
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[7,13]`
8	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[8,14]`

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

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

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

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

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

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

continued ...

Table 9

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