MSG No. 137.509 $P4_2/n'mc$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-4'm2'`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4'm2'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2mm.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `2mm.`

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

Table 5: Wyckoff site: `8e`, site symmetry: `-1'`

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

continued ...

Table 5

No.	position	mapping
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[7,11]
8	$\left[0, 0, \frac{1}{2}\right]$	[8,12]

Table 6: Wyckoff site: 8f, site symmetry: ..2'

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

Table 7: Wyckoff site: 8g, site symmetry: .m.

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

Table 8: Wyckoff site: 16h, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[\frac{1}{2}-y, x, z+\frac{1}{2}\right]$	[2]
3	$\left[y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[3]
4	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	[4]
5	$\left[\frac{1}{2}-x, y, z\right]$	[5]
6	$\left[x, \frac{1}{2}-y, z\right]$	[6]
7	$\left[\frac{1}{2}-y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[7]
8	$\left[y, x, z+\frac{1}{2}\right]$	[8]
9	$\left[x+\frac{1}{2}, -y, -z\right]$	[9]

continued ...

Table 8

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