MSG No. 67.501 $Cmma$ [Type I, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222`

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `.2/m.`

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

continued ...

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `.2/m.`

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm2`

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

Table 8: Wyckoff site: `8h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `8i`, site symmetry: `2..`

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1,2]`
2	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[3,4]`
3	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[5,6]`

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: .2.

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

Table 11: Wyckoff site: 8k, site symmetry: .2.

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

Table 12: Wyckoff site: 8l, site symmetry: ..2

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

continued ...

Table 12

No.	position	mapping
7	$\left[\frac{1}{4}, \frac{1}{2}, -z\right]$	[13,16]
8	$\left[\frac{1}{4}, \frac{1}{2}, z\right]$	[14,15]

Table 13: Wyckoff site: 8m, site symmetry: m..

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

Table 14: Wyckoff site: 8n, site symmetry: .m.

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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

continued ...

Table 15

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