MSG No. 66.491 $Cccm$ [Type I, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: `8l`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,8]`
2	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[2,7]`
3	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[3,6]`

continued ...

Table 12

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

Table 13: Wyckoff site: `16m`, site symmetry: `1`

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