MSG No. 58.404 P_Innm [Type IV, orthorhombic]

Table 1: Wyckoff site: `2a`, site symmetry: `m'm'm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `m'm'm`

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

Table 3: Wyckoff site: `2c`, site symmetry: `m'm'm`

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

Table 4: Wyckoff site: `2d`, site symmetry: `m'm'm`

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `m'2'm`

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

Table 8: Wyckoff site: `4h`, site symmetry: `m'2'm`

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

Table 9: Wyckoff site: `4i`, site symmetry: `m'm'2`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m'm'2`

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

Table 11: Wyckoff site: `8k`, site symmetry: `-1'`

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

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

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

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

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

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

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

continued ...

Table 14

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

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

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