MSG No. 12.64 C_a2/m [Type IV, monoclinic]

Table 1: Wyckoff site: `4a`, site symmetry: `2/m`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2/m'`

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

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

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,3,4]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[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: `2'/m`

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

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

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[3,5,12,14]`
4	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[4,6,11,13]`

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

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

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

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

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

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

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

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

continued ...

Table 9

No.	position	mapping
8	$\left[0,\ \frac{1}{2}-y,\ 0\right]$	`[15,16]`

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

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

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

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

Table 12: Wyckoff site: `8l`, site symmetry: `2'`

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

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

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

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

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

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

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