MSG No. 12.63 C_c2/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	$\left[0, 0, \frac{1}{2}\right]$	`[9,10,11,12]`
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[13,14,15,16]`

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

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

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

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

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

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

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

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

continued ...

Table 5

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

Table 6: Wyckoff site: `8f`, site symmetry: `-1'`

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

Table 7: Wyckoff site: `8g`, 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	$\left[0, y, \frac{1}{2}\right]$	[9,10]
6	$\left[0, -y, \frac{1}{2}\right]$	[11,12]
7	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	[13,14]
8	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}\right]$	[15,16]

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: `8i`, 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	$\left[x, 0, z + \frac{1}{2}\right]$	[9,12]
6	$\left[-x, 0, \frac{1}{2} - z\right]$	[10,11]
7	$\left[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[13,16]
8	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} - z\right]$	[14,15]

Table 10: Wyckoff site: `16j`, 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	$\left[x, y, z + \frac{1}{2}\right]$	[9]
10	$\left[-x, y, \frac{1}{2} - z\right]$	[10]
11	$\left[-x, -y, \frac{1}{2} - z\right]$	[11]
12	$\left[x, -y, z + \frac{1}{2}\right]$	[12]
13	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[13]
14	$\left[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[14]
15	$\left[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[15]
16	$\left[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[16]