MSG No. 63.463 $Cmc'm'$ [Type III, orthorhombic]

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4]`
2	$\left[0, 0, \frac{1}{2}\right]$	`[5,6,7,8]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[5,6,7,8]`
3	$\left[\frac{1}{2}, 0, 0\right]$	`[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: `m2'm'`

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

Table 4: Wyckoff site: `8d`, site symmetry: `-1`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2..`

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

Table 6: Wyckoff site: `8f`, site symmetry: `m..`

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

Table 7: Wyckoff site: `8g`, site symmetry: `..m'`

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

Table 8: Wyckoff site: `16h`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[-x, -y, -z]$	[3]

continued ...

Table 8

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